Mean force Gibbs state and steady states of quantum master equations

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- System + Bath + Interaction

$$H = H_{\mathrm{S}} + H_{\mathrm{B}} + H_{\mathrm{I}},$$

with

$$H_{\mathrm{I}} = \epsilon \sum_{\alpha} A_\alpha \otimes B_\alpha,$$

- Reduced density operator

$$\rho(t) = \mathrm{Tr}_{\mathrm{B}}(e^{-iHt}(\rho(0) \otimes \rho_B)e^{iHt}) = \mathcal{E}_{(t,0)}[\rho(0)],$$

with $\rho_{\mathrm{B}} = e^{-\beta H_{\mathrm{B}}}/Z_{\mathrm{B}}$.

- (Time-local) Quantum master equations

$$\frac{d\rho(t)}{dt} = \mathcal{L}[\rho(t)].$$

- Weak coupling master equations ($O(\epsilon^2)$)
- Born-Markov approximation
- Redfield equation
  - Obtained from formal perturbation (TCL projection operator formalism)
  - Does not guarantee positivity
- Davies equation
  - Secular approximation
  - Lindblad form: CP
- Recent CP master equations which do not rely on secular approximation
  - Universal Lindblad equation (ULE) [Nathan and Rudner, PRB **102**, 115109 (2020)]
  - Truncated Lindblad equation (TLE) [Becker et al. PRE **104**, 014110 (2021)]
  - Obtained by modifying Redfield equation to achieve Lindblad form

Introduction

Steady states of QMEs

- Steady state ($\rho(t) \to \rho^{\rm st}$ as $t \to \infty$) of $d\rho(t)/dt = \mathcal{L}[\rho(t)]$

$$\mathcal{L}[\rho^{\rm st}] = 0$$

- If the total system thermalizes, we expect $\rho_{\rm s} = \rho_{\rm mG}$, mean-force Gibbs state

$$\rho_{\rm mG} \equiv \frac{{\rm Tr}_{\rm B}(e^{-\beta H})}{{\rm Tr}_{\rm SB}(e^{-\beta H})}.$$

- Weak coupling limit

$$\rho_{\rm mG} = \rho_{\rm G} + \epsilon^2 \rho_{\rm mG}^{(2)} + \cdots , \qquad \rho_{\rm G} = \frac{e^{-\beta H_{\rm S}}}{Z_{\rm S}}$$

- What we did: Calculate $\rho^{\rm st}$ of various QMEs perturbatively

$$\rho^{\rm st} = \rho^{(0)} + \epsilon^2 \rho^{(2)} + \cdots$$

and compare with $\rho_{\rm mG}$.

Perturbative Steady State of QME

- Generic weak coupling QMEs

$$\frac{d\rho(t)}{dt} = \mathcal{L}^{(0)}[\rho(t)] + \epsilon^2 \mathcal{L}^{(2)}[\rho(t)] + O(\epsilon^4)$$

  with

$$\mathcal{L}^{(0)}[\rho(t)] = -i[H_S, \rho(t)]$$

- With $\rho^{\rm st} = \rho^{(0)} + \epsilon^2 \rho^{(2)} + O(\epsilon^4)$, we have

$$O(\epsilon^0): \ \mathcal{L}^{(0)}[\rho^{(0)}] = 0, \qquad O(\epsilon^2): \ \mathcal{L}^{(0)}[\rho^{(2)}] + \mathcal{L}^{(2)}[\rho^{(0)}] = 0$$

- Matrix elements: $\rho_{nm} = \langle n|\rho|m\rangle$ with $H_{\rm S}|n\rangle = E_n|n\rangle$

$$-i\Delta_{nm}\rho^{(0)}_{nm} = 0 \qquad \Rightarrow \qquad \boxed{\rho^{(0)}_{nm} = 0} \qquad \text{for} \quad n \neq m,$$

$$-i\Delta_{nm}\rho^{(2)}_{nm} + \left(\mathcal{L}^{(2)}[\rho^{(0)}]\right)_{nm} = 0, \qquad \text{where} \quad \Delta_{nm} = E_n - E_m$$

Perturbative Steady State of QME

2nd order coherence and population

0th-order: $n = m$

$$\left(\mathcal{L}^{(2)}[\rho^{(0)}]\right)_{nn} = 0 \qquad \Rightarrow \text{detemines} \qquad \rho^{(0)}_{nn} \qquad (\star)$$

2nd-order coherence: $n \neq m$

$$\rho^{(2)}_{nm} = \frac{1}{i\Delta_{nm}}\left(\mathcal{L}^{(2)}[\rho^{(0)}]\right)_{nm} \qquad (\star\star)$$

- 2nd order population $\rho^{(2)}_{nn}$ is not determined to this order. We need $\mathcal{L}^{(4)}$.
- Method of analytic continuation [Thingna et al, J. Chem. Phys. **136**, 194110 (2012)]
  – If the limit $n \to m$ exists in $(\star\star)$, we may regard this as $\rho^{(2)}_{nn}$

Redfield equation

- Born-Markov approximation (interaction picture)

$$\frac{d\tilde{\rho}(t)}{dt} = -\int_0^{\infty} ds\, \mathrm{Tr}_\mathrm{B}[\tilde{H}_\mathrm{I}(t), [\tilde{H}_\mathrm{I}(t-s), \underset{\sim\sim\sim}{\tilde{\rho}(t)\otimes\rho_\mathrm{B}}]].$$

- (Schrödinger picture) With $A_\alpha(\omega) \equiv \sum_{m,n,E_n-E_m=\omega} |m\rangle\langle m|A_\alpha|n\rangle\langle n|$

$$\mathcal{L}^{(2)}_\mathrm{Red}[\rho(t)] = -\sum_{\alpha,\beta}\sum_{\omega,\omega'}\Big(\Gamma_{\alpha\beta}(\omega)[A^\dagger_\alpha(\omega'), A_\beta(\omega)\rho(t)] + \mathrm{h.c.}\Big),$$

- Bath correlation function ($\tilde{B}_\alpha(t) \equiv e^{iH_B t}B_\alpha e^{-iH_B t}$)

$$\Gamma_{\alpha\beta}(\omega) \equiv \int_0^\infty ds\, e^{i\omega s}C_{\alpha\beta}(s), \qquad C_{\alpha\beta}(t) \equiv \mathrm{Tr}_B[\tilde{B}_\alpha(t)B_\beta\rho_B]$$

Define

$$\gamma_{\alpha\beta}(\omega) \equiv \Gamma_{\alpha\beta}(\omega) + \Gamma^*_{\beta\alpha}(\omega) = \int_{-\infty}^\infty ds\, e^{i\omega s}C_{\alpha\beta}(s)$$

$$S_{\alpha\beta}(\omega) \equiv \frac{1}{2i}(\Gamma_{\alpha\beta}(\omega) - \Gamma^*_{\beta\alpha}(\omega))$$

Steady state of Redfield equation

- Write

$$\mathcal{L}_{\rm Red}^{(2)} = \mathcal{L}_{\rm Red}^{(S)} + \mathcal{L}_{\rm Red}^{(\gamma)}$$

- $(\mathcal{L}_{\rm Red}^{(S)}[\rho^{(0)}])_{nn} = 0$ automatically if $\rho^{(0)}$ is diagonal. Eq. $(\star)$ becomes

$$0 = \left(\mathcal{L}_{\rm Red}^{(\gamma)}[\rho^{(0)}]\right)_{nn} = \sum_{\alpha,\beta}\sum_{j}\left(\gamma_{\alpha\beta}(\Delta_{jn})\rho_{jj}^{(0)} - \gamma_{\beta\alpha}(\Delta_{nj})\rho_{nn}^{(0)}\right)(A_\beta)_{nj}(A_\alpha)_{jn}$$

- KMS (equilibrium) condition for bath: $\gamma_{\alpha\delta}(-\omega) = e^{-\beta\omega}\gamma_{\delta\alpha}(\omega)$

$$\rho^{(0)} = \rho_{\rm G}$$

Steady state of Redfield equation

2nd order contribution

- Because of $\mathcal{L}_{\mathrm{Red}}^{(S)}$ part, $\rho^{\mathrm{st}} \neq \rho_{\mathrm{G}}$
- 2nd order coherence: (using $(\star\star)$ with $(\mathcal{L}_{\mathrm{Red}}^{(\gamma)}[\rho_{\mathrm{G}}])_{nm} = 0$)

$$\rho_{nm}^{(2)} = \frac{1}{\Delta_{nm}} \sum_{\alpha,\beta,j} \Big[\{S_{\beta\alpha}(\Delta_{jn}) - S_{\beta\alpha}(\Delta_{jm})\}\rho_{jj}^{(0)} + \Big\{ S_{\alpha\beta}(\Delta_{nj})\rho_{nn}^{(0)} - S_{\alpha\beta}(\Delta_{mj})\rho_{mm}^{(0)} \Big\} \Big] (A_\alpha)_{nj}(A_\beta)_{jm}.$$

- Analytic continuation to get

$$\bar{\rho}_{nn}^{(2)} = \sum_{\alpha,\mu,j} \Big[-S'_{\mu\alpha}(\Delta_{jn})\rho_{jj}^{(0)} + S'_{\alpha\mu}(\Delta_{nj})\rho_{nn}^{(0)} - \beta S_{\alpha\mu}(\Delta_{nj})\rho_{nn}^{(0)} \Big] (A_\alpha)_{nj}(A_\mu)_{jn}.$$

- After normalization, 2nd order population is

$$\rho_{nn}^{(2)} = \bar{\rho}_{nn}^{(2)} - \rho_{nn}^{(0)} \sum_k \bar{\rho}_{kk}^{(2)}$$

Steady state of Redfield equation

Comparison with MFG state

- Recall $\rho_{\rm mG} \equiv {\rm Tr}_{\rm B}(e^{-\beta(H_{\rm S}+H_{\rm I}+H_{\rm B})})/Z$
- With $\rho_{\rm mG} = \rho_{\rm G} + \epsilon^2 \rho^{(2)}_{\rm mG} + \cdots$,

$$\rho^{(2)}_{\rm mG} = \frac{\mathcal{D}}{Z_{\rm S}} - \frac{{\rm Tr}_{\rm S}(\mathcal{D})}{Z_{\rm S}^2} e^{-\beta H_{\rm S}}$$

where

$$\mathcal{D} = \int_0^\beta d\lambda_1 \int_0^{\lambda_1} d\lambda_2 \; e^{-\beta H_{\rm S}} \sum_{\alpha,\gamma} \tilde{A}_\alpha(-i\lambda_1)\tilde{A}_\gamma(-i\lambda_2) C_{\alpha\gamma}(-i(\lambda_1-\lambda_2))$$

- One can show that [Thingna et al, J. Chem. Phys. **136**, 194110 (2012)]

$$\frac{\mathcal{D}_{nm}}{Z_{\rm S}} = \rho^{(2)}_{nm} \quad for \quad n \neq m, \qquad \frac{\mathcal{D}_{nn}}{Z_{\rm S}} = \bar{\rho}^{(2)}_{nn}$$

- In the high temperature limit

$$\rho_{\rm mG} = \rho_{\rm G} + \text{ higher order than } \epsilon^2.$$

Secular approximation and the Lindblad form

- Secular approximation: Take $\omega = \omega'$ term in

$$\frac{d\tilde{\rho}(t)}{dt} = -\epsilon^2 \sum_{\alpha,\beta} \sum_{\omega,\omega'} \left(e^{i(\omega'-\omega)t} \Gamma_{\alpha\beta}(\omega) [A^\dagger_\alpha(\omega'), A_\beta(\omega)\tilde{\rho}(t)] + \mathrm{h.c.} \right)$$

  - Valid when $|\omega - \omega'| \gg t^{-1}$. Since $t \gg \tau_{\mathrm{B}}$, it means $\min|\omega - \omega'| > \tau_{\mathrm{B}}^{-1}$
  - It breaks down when there are energy gaps small than τ_{B}^{-1}
  - Equivalent to Davies theory: rescaled time $\tau \equiv \epsilon^2 t$ in the limit $\epsilon \to 0$ with finite τ

- S-part becomes unitary evolution

$$\mathcal{L}^{(S)}_{\mathrm{sec}}[\rho(t)] = -i[H_{\mathrm{LS}}, \rho(t)], \qquad H_{\mathrm{LS}} = \sum_{\alpha,\beta} \sum_{\omega} S_{\alpha\beta}(\omega) A^\dagger_\alpha(\omega) A_\beta(\omega)$$

- γ-part takes the Lindblad form ($\gamma_{\alpha\beta}$ is positive definite)

$$\mathcal{L}^{(\gamma)}_{\mathrm{sec}}[\rho(t)] = \sum_{\alpha,\beta} \sum_{\omega} \gamma_{\alpha\beta}(\omega) \Big(A_\beta(\omega)\rho(t)A^\dagger_\alpha(\omega) - \frac{1}{2} \left\{ A^\dagger_\alpha(\omega) A_\beta(\omega), \rho(t) \right\} \Big).$$

Steady state of Davies equation

- Recall that KMS condition gives $\mathcal{L}^{(\gamma)}_{\rm Red}[\rho_{\rm G}] = 0$.
- Similarly, we have
$$\mathcal{L}^{(\gamma)}_{\rm sec}[\rho_{\rm G}] = 0$$
- Unlike Redfield equation, $\mathcal{L}^{(S)}_{\rm sec}$ now takes the form of the unitary evolution. We have
$$\mathcal{L}^{(S)}_{\rm sec}[\rho_{\rm G}] = 0$$
using $A^\dagger_\alpha(\omega)A_\beta(\omega)\rho_{\rm G} = \rho_{\rm G}A^\dagger_\alpha(\omega)A_\beta(\omega)$.
- For Davies equation
$$\rho^{\rm st} = \rho_{\rm G} + O(\epsilon^4)$$
- Although equation itself is of $O(\epsilon^2)$, the steady state does not contain the effect of the coupling to bath to this order. $\Rightarrow$ Ultraweak coupling theory

Universal Lindblad equation (ULE)

[Nathan and Rudner, PRB **102**, 115109 (2020)]

- Does not rely on the secular approximation
- Has the same level of accuracy as the Redfield equation.
- The main ingredient of the approximation is the identification of a small parameter given in terms of the properties of the bath valid in the weak-coupling limit.
- $\partial_t \rho(t) = \mathcal{L}^{(0)}[\rho(t)] + \epsilon^2 \mathcal{L}^{(2)}_{\mathrm{ULE}}[\rho(t)]$

$$\mathcal{L}^{(2)}_{\mathrm{ULE}} = \mathcal{L}^{(a)}_{\mathrm{ULE}} + \mathcal{L}^{(b)}_{\mathrm{ULE}}$$

- $\mathcal{L}^{(a)}_{\mathrm{ULE}}[\rho(t)] = -i[\Lambda, \rho(t)]$ with

$$\Lambda = \sum_{\alpha,\beta} \sum_{\omega,\omega'} f_{\alpha\beta}(\omega,\omega') A_\alpha(\omega) A_\beta(\omega'),$$

- Dissipator in the Lindblad form

$$\mathcal{L}^{(b)}_{\mathrm{ULE}}[\rho(t)] = \sum_\alpha [L_\alpha \rho(t) L_\alpha^\dagger - \frac{1}{2}\{L_\alpha^\dagger L_\alpha, \rho(t)\}]$$

More on ULE

- Here the jump operator is

$$L_\alpha = \sum_\beta \sum_\omega g_{\alpha\beta}(\omega) A_\beta(\omega), \qquad \text{with} \qquad \gamma_{\alpha\beta}(\omega) = \sum_\mu g_{\alpha\mu}(\omega) g_{\mu\beta}(\omega).$$

- Compare with

$$\mathcal{L}^{(\gamma)}_{\text{sec}}[\rho(t)] = \sum_{\alpha,\beta} \sum_\omega \gamma_{\alpha\beta}(\omega) \Big(A_\beta(\omega)\rho(t)A^\dagger_\alpha(\omega) - \frac{1}{2}\Big\{ A^\dagger_\alpha(\omega)A_\beta(\omega), \rho(t) \Big\} \Big).$$

- Since $\gamma_{\alpha\beta}(\omega)$ is positive semidefinite, $g_{\alpha\beta}(\omega)$ is hermitian and also positive semidefinite.
- $f_{\alpha\beta}(\omega,\omega')$ is given by

$$f_{\alpha\beta}(\omega,\omega') \equiv -\mathcal{P} \sum_\mu \int_{-\infty}^{\infty} \frac{d\tilde{\omega}}{2\pi} \frac{1}{\tilde{\omega}} g_{\alpha\mu}(\tilde{\omega}-\omega) g_{\mu\beta}(\tilde{\omega}+\omega').$$

- Compare with

$$S_{\alpha\beta}(\omega) = -\mathcal{P} \int_{-\infty}^{\infty} \frac{d\tilde{\omega}}{2\pi} \frac{1}{\tilde{\omega}} \gamma_{\alpha\beta}(\tilde{\omega}+\omega),$$

- ULE roughly corresponds to taking the square root of the Fourier transform of the bath correlation function and to distributing it to the new jump operators.

Steady state of ULE

- From KMS condition $g_{\alpha\delta}(-\omega) = e^{-\beta\omega/2} g_{\delta\alpha}(\omega)$, we again have

$$\rho^{(0)} = \rho_{\mathrm{G}}$$

- 2nd order coherence

$$\rho^{(2)}_{nm} = \frac{1}{i\Delta_{nm}} \Bigg[-i \sum_{\alpha,\beta} \sum_{k} f_{\alpha\beta}(\Delta_{kn}, \Delta_{mk}) (A_\alpha)_{nk} (A_\beta)_{km} \left(\rho^{(0)}_{mm} - \rho^{(0)}_{nn} \right)$$

$$+ \sum_{\alpha,\beta,\gamma} \sum_{k} (A_\beta)_{nk} (A_\gamma)_{km} \Big\{ g_{\alpha\beta}(\Delta_{kn}) g_{\gamma\alpha}(\Delta_{km}) \rho^{(0)}_{kk} - \frac{1}{2} g_{\beta\alpha}(\Delta_{nk}) g_{\alpha\gamma}(\Delta_{mk}) \left(\rho^{(0)}_{mm} + \rho^{(0)}_{nn} \right) \Big\} \Bigg]$$

- 2nd order population

$$\bar{\rho}^{(2)}_{nn} = -\beta \sum_{\alpha,\delta,k} f_{\alpha\delta}(\Delta_{kn}, \Delta_{nk}) (A_\alpha)_{nk} (A_\delta)_{kn} \rho^{(0)}_{nn}.$$

- These are manifestly different from $\rho^{(2)}_{\mathrm{mG}}$.

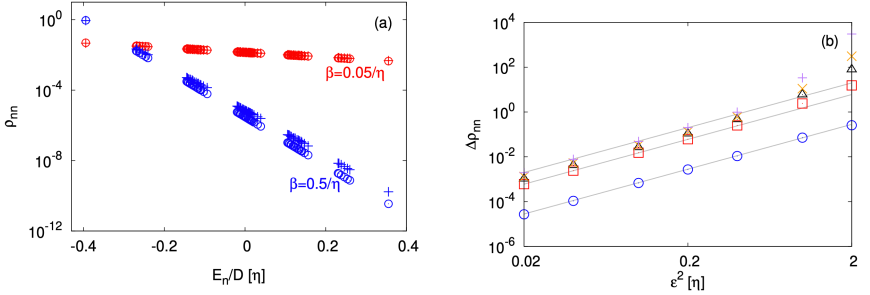
Example 1

Steady state of spin chain

- A bath is coupled to $i = 1$ spin through S_1^x with a coupling strength ϵ

$$H_{\rm S} = -B_z \sum_{i=1}^{N} \sigma_i^z - \eta \sum_{i=1}^{N-1} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_{i+1},$$

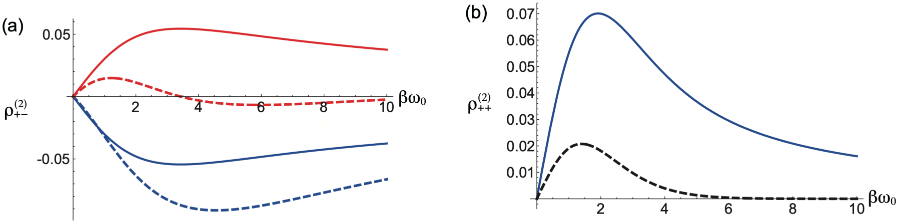
- Numerically follow the evolution through ULE
- Term with $f(\omega, \omega')$ is not used.
- $\circ = (\rho_{\rm G})_{nn}$, $+ = \rho_{nn}^{\rm st}$; Difference is of $O(\epsilon^4)$



- System $H_{\rm S} = (\omega_0/2)\sigma_z$ is coupled with a bath of harmonic oscillators $H_{\rm B} = \sum_k \omega_k a_k^\dagger a_k$ via

$$H_{\rm I} = (c_x\sigma_x + c_y\sigma_y + c_z\sigma_z)\sum_k \frac{\lambda_k}{2}(a_k^\dagger + a_k),$$

- Solid lines = MFG state; Dashed lines = SS of ULE



Truncated Lindblad equation

Becker et al. PRE **104**, 014110 (2021)

- Rewrite Redfield equation in the form

$$\frac{d\rho}{dt} = -i[H_{\rm S} + H_{\rm LS}, \rho] + \epsilon^2 \mathcal{D}_{\rm Red},$$

with

$$H_{\rm LS} = \frac{\epsilon^2}{2i}(A\mathbb{A}_t - \mathbb{A}_t^\dagger A)$$

$$\mathcal{D}_{\rm Red} = A\rho\mathbb{A}_t^\dagger + \mathbb{A}_t\rho A - \frac{1}{2}\left\{A\mathbb{A}_t + \mathbb{A}_t^\dagger A, \rho\right\}$$

where

$$\mathbb{A}_t = \int_0^t d\tau\, C(\tau) e^{-iH_{\rm S}\tau} A e^{iH_{\rm S}\tau}$$

More on TLE

- We can write

$$\mathcal{D}_{\rm Red} = \mathcal{D}_{+} - \mathcal{D}_{-}$$

- Throw away the negative contribution from the Redfield equation

$$\frac{d\rho}{dt} = -i[H_{\rm S} + H_{\rm LS}, \rho] + \epsilon^2 \mathcal{D}_{+},$$

where

$$\mathcal{D}_{\pm} = L_{\pm}\rho L_{\pm}^{\dagger} - \frac{1}{2}\{L_{\pm}^{\dagger}L_{\pm}, \rho\}.$$

and

$$L_{\pm} = \frac{1}{\sqrt{2\cos\varphi_t}}\left(\lambda_t^{\pm} A + \frac{1}{\lambda_t^{\pm}}\mathbb{A}_t\right).$$

- $\mathcal{D}_{-}$ part is thrown away; Freedom to choose λ_t and φ_t to minimize the truncated part.
- We found that the zeroth order steady state $\boxed{\rho^{(0)} \neq \rho_{\rm G}}$.

Summary and Conclusion

	CP	$\rho^{(0)}$	$\rho^{(2)}$
Redfield	No	ρ_{G}	$\rho^{(2)}_{\mathrm{mG}}$
Davies (Secular Approx.)	Yes	ρ_{G}	0
ULE	Yes	ρ_{G}	$\neq \rho^{(2)}_{\mathrm{mG}}$
TLE	Yes	$\neq \rho_{\mathrm{G}}$	$\neq \rho^{(2)}_{\mathrm{mG}}$

- We have explicitly calculated, in a perturbative manner, the equilibrium steady states of recently developed Lindbladian QMEs.
- We have compared the results with the steady state of the Redfield equation obtained from an analytic continuation method, which coincides with MFG state.
- We found that manipulations of the Redfield equation needed to enforce CP of a QME drives its steady state away from the MFG state.
- In the high-temperature regime, both the steady states of the Lindbladian QMEs and MFG state reduce to the system Gibbs state