Dynamics for a small quantum system open to a bath with thermostat

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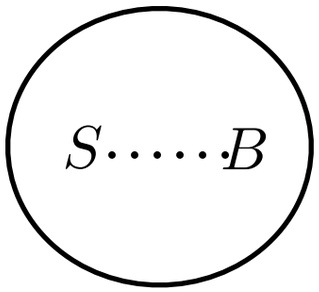
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I. Outline

Previous weak coupling theory



isolated

$\dot{\rho}_{SB} = -i[H_I, \rho_{SB}]$ unitary

$$\dot{\rho}_S = -\mathrm{Tr}_B \int_0^t dt' \left[H_I(t) \left[H_I(t'), \rho_{SB}(t')\right]\right]$$

weak coupling between S & B

$\rho_{SB}(t') \simeq \rho_S(t') \otimes e^{-\beta H_B}$ Born approx

$\mathrm{Tr}_B O_B(t) O_B(t') e^{-\beta H_B}$ fast dissipating

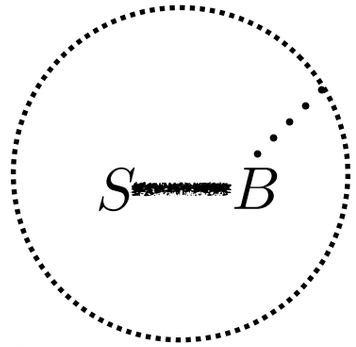
$\rho_S(t') \simeq \rho_S(t)$ Markov approx

$\dot{\rho}_S = \mathcal{L}_S^{\mathrm{RF}}[\rho_S]$ Redfield eq

$\rho_S^{ss} = \mathrm{Tr}_B e^{-\beta(H_S+H_B+H_I)}$ yes or no?

mean for Gibbs (MFG)

Our approach

open 

SU(super bath)

$$\dot{\rho} = -i\left[H_I + H_{I-BSU}, \rho\right]$$

weak coupling between B & SU

non-unitary $\dot{\rho}_{SB} = -i[H_I, \rho_{SB}] + \mathcal{L}_B^X[\rho_{SB}]$

$$\dot{\rho}_S = -\mathrm{Tr}_B \int_0^t dt' \left[H_I(t) \left[H_I(t'), \rho_{SB}(t')\right]\right]$$
$$-i\mathrm{Tr}_B \int_0^t dt' \left[H_I(t), \mathcal{L}_B^X[\rho_{SB}(t')\right]$$
$$+\mathrm{Tr}_B \mathcal{L}_B^X[\rho_{SB}(t)]$$

strong coupling between S & B

rigorous perturbation theory

...

...

$\dot{\rho}_S = \widetilde{\mathcal{L}}_S^{\mathrm{RF}}[\rho_S]$

ρ_S^{ss} is definitely not MFG state.

II. Photonic bath interacting with Caldeira-Legett super bath

Following the text book by Breuer & Petruccione,"The theory of open quantum systems"

1. Photonic bath

$$H_{\mathrm{B}} = \sum_{\mathbf{k}\lambda} \hbar\omega_{\mathbf{k}} b^{\dagger}_{\mathbf{k}\lambda} b_{\mathbf{k}\lambda}$$

2nd quantized electric field

$$\mathbf{E}(\mathbf{r}) = i\sqrt{\frac{2\pi\hbar}{V}} \sum_{\mathbf{k}\lambda} \sqrt{\omega_{\mathbf{k}}}\mathbf{e}_{\mathbf{k}\lambda} \left[b_{\mathbf{k}\lambda} e^{i\mathbf{k}\cdot\mathbf{r}} - b^{\dagger}_{\mathbf{k}\lambda} e^{-i\mathbf{k}\cdot\mathbf{r}} \right] ,$$

2. Caldera-Legett (CL) SU

- Collection of infinitely many harmonic oscillators with dipole moments

$$H_{SB} = \sum_{n=1}^{N\to\infty} \hbar\omega_n c^{\dagger}_n c_n$$

$$\mathbf{p}_n = \mathbf{d}_n q_n x_n = \mathbf{d}_n \kappa_n (c_n + c^{\dagger}_n) \qquad \text{where } \kappa_n = \sqrt{\frac{\hbar q_n^2}{m_n \omega_n}}$$

3. Interaction between B and SU

$$H_{I-BSU} = -\sum_n \mathbf{p}_n \cdot \mathbf{E}(\mathbf{r}_n) = -\sum_{n,a} \kappa_n \hat{p}^a_n (c_n + c^{\dagger}_n) E^a_n$$

Eigen-operator

$$E^a_n(\omega > 0) = i\sqrt{\frac{2\pi\hbar\omega}{V}} \sum_{\mathbf{k}\in S_\omega, \lambda} e^a_{\mathbf{k}\lambda} b_{\mathbf{k}\lambda} e^{i\mathbf{k}\cdot\mathbf{r}_n} \qquad E^a_n(\omega < 0) = E^a_n(|\omega|)^{\dagger}$$

$$S_\omega : \text{ spherical surface with } k = \omega/c$$

4. Dissipator of Lindblad type

$$\Gamma^{ab}_{nm}(\omega) = \int_0^\infty dt e^{i\omega t}\langle p^a_n(t)p^b_m(0)\rangle_{SU}$$

$$= \kappa_n\kappa_m d^a_n d^b_m \int_0^\infty dt e^{i\omega t} \underbrace{\langle (c_n e^{-i\omega_n t} + c^\dagger_m e^{i\omega_n t})(c_m + c^\dagger_m)\rangle}_{\delta_{nm}((N(\omega_n)+1)e^{-i\omega_n t} + N(\omega_n)e^{i\omega_n t})}$$

$$= \delta_{nm}\pi\kappa_n^2\ \hat{p}^a_n\hat{p}^b_n\ \ [(N(\omega_n)+1)\delta(\omega-\omega_n) + \pi N(\omega_n)\delta(\omega+\omega_n)]$$

$$\text{where} \int_0^\infty dt e^{i(\omega-\omega_n)t} = \pi\delta(\omega-\omega_n) + iP\frac{1}{\omega-\omega_n} \qquad , N(\omega) = \frac{1}{e^{\beta\hbar\omega}-1}$$

$$\Gamma^{ab}_{nn}(\omega)E^a_n(\omega)\rho_{SB}E^b_n(\omega)^\dagger =$$

$$\sum_{\omega>0}\sum_{a,b}\sum_{n=1}^{N}\frac{q_n^2}{m_n\omega_n}(N(\omega_n)+1)d^a_n d^b_n\frac{2\pi\omega}{V}\sum_{\mathbf{k}\lambda}\sum_{\mathbf{k}'\lambda'}\delta(\omega-\omega_n)e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}_n}\hat{e}^a_{\mathbf{k}\lambda}\hat{e}^b_{\mathbf{k}'\lambda'}b_{\mathbf{k}\lambda}\ \rho_{\mathrm{SB}}\ b^\dagger_{\mathbf{k}'\lambda'}$$

$$e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}_n} \to \delta_{\mathbf{k}\mathbf{k}'} \quad \text{fast oscillating for } |\mathbf{r}_n| \to \infty$$

$\{\omega_n\}$ almost continuous for $N\to\infty$ and $\omega_n < \omega_c$ (cut-off)

In small window $d\omega$, still many frequencies are distributed.

randomly oriented dipoles $$\sum_{\omega_n\in[\omega,\omega+d\omega]}\frac{q_n^2}{m_n\omega_n}\underbrace{d^a_n d^b_n}_{\delta_{ab}/3}\delta(\omega-\omega_n)$$

Orthogonal polarization basis $$\sum e^a_{\mathbf{k}\lambda}e^a_{\mathbf{k}\lambda'} = \mathbf{e}_{\mathbf{k}\lambda}\cdot\mathbf{e}_{\mathbf{k}\lambda'} = \delta_{\lambda\lambda'}$$

Spectral density $$J(\omega) = \frac{1}{N}\sum_{\omega_n}^{a}\frac{q_n^2}{m_n\omega_n}\delta(\omega-\omega_n)$$

$$\mathcal{L}_{\mathrm{B}}^{\mathrm{LB}}[\rho_{SB}]=\sum_{\mathbf{k},\lambda}\mu(\omega)\Big[(N(\omega)+1)\left(b_{\mathbf{k}\lambda}\rho_{SB}b_{\mathbf{k}\lambda}^{\dagger}-\frac{1}{2}\left\{b_{\mathbf{k}\lambda}^{\dagger}b_{\mathbf{k}\lambda},\rho_{SB}\right\}\right)+N(\omega)\left(b_{\mathbf{k}\lambda}^{\dagger}\cdot b_{\mathbf{k}\lambda}-\frac{1}{2}\left\{b_{\mathbf{k}\lambda}b_{\mathbf{k}\lambda}^{\dagger},\rho_{SB}\right\}\right)\Big]$$

where

$$\begin{aligned}\mu(\omega) &= \frac{\pi}{3}\frac{N}{V}\omega J(\omega)\\ &= \frac{\pi}{3a_0^2V^{1/3}}\omega J(\omega) \quad \text{where } N=\frac{V^{2/3}}{a_0^2} \text{ for average spacing } a_0\\ &= \omega_0\mu_0\frac{\omega}{\omega_0}\frac{\pi J(\omega)}{3a_0^2V^{1/3}}\\ &= \omega_0\bar{\mu}(\omega)\end{aligned}$$

– Dissipator of each photon mode $\sim \frac{1}{V}\times$ number of CL oscillators $\sim V^{-1/3}$

– $\mu(\omega)$ is very small in thermodynamic limit.

–One can use the Redfield-type dissipator $\mathcal{L}_B^{\mathrm{RF}}$

III. Strongly coupled system and bath

1. Dipole interaction between S and optical B

$$H_{\mathrm{I}} = -\mathbf{p}\cdot\mathbf{E}(\mathbf{r}=\mathbf{0}) = -i\sum_{\mathbf{k}\lambda}\sqrt{\frac{2\pi\hbar\omega}{V}}\sum_{\alpha} e^{\alpha}_{\mathbf{k}\lambda}p_{\alpha}(b_{\mathbf{k}\lambda}-b^{\dagger}_{\mathbf{k}\lambda})$$

2. Harmonic oscillator system

$$H_{\mathrm{S}} = \hbar\omega_0\left(aa^{\dagger}+\frac{1}{2}\right), \quad \mathbf{p} = \hat{\mathbf{x}}qx = \hat{\mathbf{x}}q\sqrt{\frac{\hbar}{2m\omega_0}}(a+a^{\dagger})$$

$$H_{\mathrm{I}} = -i\hbar\sum_{\mathbf{k},\lambda}\gamma_{\mathbf{k}\lambda}(\omega)(a+a^{\dagger})(b_{\mathbf{k}\lambda}-b^{\dagger}_{\mathbf{k}\lambda})$$

$$\text{where } \gamma_{\mathbf{k}\lambda}(\omega) = \omega_0\sqrt{\frac{\pi q^2}{m\omega_0^2 V}}\sqrt{\frac{\omega}{\omega_0}}e^{x}_{\mathbf{k}\lambda} = \omega_0\sqrt{\frac{\pi\nu}{V}}\sqrt{\frac{\omega}{\omega_0}}e^{x}_{\mathbf{k}\lambda}$$

$$\dot{\rho}_{\mathrm{SB}} = -\frac{i}{\hbar}\left[\hbar\omega_0 a^{\dagger}a + H_{\mathrm{I}},\ \rho_{\mathrm{SB}}\right] + \mathcal{L}_{\mathrm{B}}[\rho_{\mathrm{SB}}]$$

3. Coherent states for $\{a, a^{\dagger}, b_{\mathbf{k}\lambda},\ b^{\dagger}_{\mathbf{k}\lambda}\} = \{b_i, b_i^{\dagger}\}\ i = 0,1,2,\cdots$ and $i=0$ for system

$$b_i|z_i\rangle\langle z_i| = z_i|z_i\rangle\langle z_i|, \quad b_i^{\dagger}|z_i\rangle\langle z_i| = \left(\frac{\partial}{\partial z_i}+z_i^{*}\right)|z_i\rangle\langle z_i|$$

$$|z_i\rangle = e^{-|z_i|^2/2}\sum_{m_i=0}^{\infty}\frac{{z_i}^{m_i}}{\sqrt{m_i!}}|m_i\rangle$$

4. P-representation for $|u\rangle = |z, z_1, \cdots, z_i, \cdots\rangle$

$$\rho_{\rm SB} = \int dudu^* P(u,u^*)|u\rangle\langle u|$$

5. Pseudo-Fokker-Planck equation for $z_i = x_i + iy_i$

$$\dot{\rho}_{\rm SB} = -\frac{i}{\hbar}\left[\hbar\omega_0 a^\dagger a + H_{\rm I},\ \rho_{\rm SB}\right] + \mathcal{L}_{\rm B}^{\rm LB}[\rho_{\rm SB}] \text{ leads to}$$

$$\begin{aligned}\dot{P} = \Bigg[&\omega_0\left(-\frac{\partial}{\partial x_0}y_0 + \frac{\partial}{\partial y_0}x_0\right) + \sum_{i>0}\omega_i\left(-\frac{\partial}{\partial x_i}y_i + \frac{\partial}{\partial y_i}x_i\right)\\ &-\sum_{i>0}\gamma_i\left[\frac{\partial}{\partial x_i}x_0 - \frac{\partial}{\partial y_0}y_i - \frac{1}{4}\left(\frac{\partial^2}{\partial x_i\partial x_0} - \frac{\partial^2}{\partial y_i\partial y_0}\right)\right]\\ &+\sum_{i>0}\frac{\mu_i}{2}\left[\left(\frac{\partial}{\partial x_i}x_i + \frac{\partial}{\partial y_i}y_i\right) + \frac{N_i}{2}\left(\frac{\partial^2}{\partial x_i^2} + \frac{\partial^2}{\partial y_i^2}\right)\right]\Bigg] P\end{aligned}$$

$$= \partial_{\mathbf{q}}\cdot(\mathsf{F}\cdot\mathbf{q} + \mathsf{D}\cdot\partial_{\mathbf{q}})P \qquad \text{where } \ \mathbf{q} = (x, y, x_1, y_1, x_2, y_2, \cdots)^{\rm t}$$

– ∞-dim Ornstein-Uhlenbeck process,not-positive diffusion)

where $N_i = (e^{\beta\hbar\omega_i} - 1)^{-1}$ for $\omega_i = c|\mathbf{k}|$

$$\gamma_i = \omega_0\sqrt{\frac{\pi\nu}{V}}\sqrt{\frac{\omega_i}{\omega_0}}e^x_{\mathbf{k}\lambda}, \quad \mu_i = \omega_0\frac{\omega_i}{\omega_0}\frac{\pi^2 J(\omega_i)}{3a_0^2 V^{1/3}}$$

6. Orders of magnitude

$q = 4.8 \times 10^{-10}$esu(electron's charge), $m = 1.7 \times 10^{-24}$g (reduced mass of H_2),

$\omega_0 \sim 10^{13}$-10^{14}s^{-1} for typical diatomic atoms, $V^{1/3} \sim 10^1$-10^2cm

$$\bar{\gamma}_{\mathbf{k}\lambda} = \omega_0^{-1}\gamma_{\mathbf{k}\lambda} = e^x_{\mathbf{k}\lambda}\left[\frac{\pi q^2}{m\omega_0^2 V}\frac{\omega}{\omega_0}\right]^{1/2} = e^x_{\mathbf{k}\lambda}\left[\frac{\pi\nu}{V}\frac{\omega}{\omega_0}\right]^{1/2} \ll 1$$

$$\bar{\mu}(\omega) = \omega_0^{-1}\mu(\omega) = \frac{\pi J(\omega)}{3a_0^2 V^{1/3}}\frac{\omega}{\omega_0}$$

$$= \frac{2\pi(\omega/\omega_0)^2}{3\omega_c/\omega_0}\overline{\left(\frac{q_n^2}{m_n\omega_n}\right)}\frac{1}{\omega_c a_0^2 V^{1/3}} \ll 1 \qquad \text{(Ohmic: } J(\omega) = C\omega\text{)}$$

(1) $\dfrac{d_{\mathbf{k}\lambda}}{\mu(\omega)} \sim \left[\dfrac{m\omega_0^2 a_0^4}{q^2 V^{1/3}}\right]^{1/2} \ll 1$ – series expansion for small d_i, treating μ_i exact

– take $\bar{\mu}_i \to 0$ limit at the end of expansion

7. Separation of time scales, *fast and slow*

– Relaxation (dissipation) factor: $e^{-\mathsf{F}t}$

– Relaxation rates (inverse of relaxation times) : real parts of eigenvalues of F

– From series expansion for eigenvalues of F

Relaxation rates: $\tau_B^{-1} \propto \omega_0\bar{\mu}_i$ (per bath mode), $\tau_S^{-1} \propto \omega_0\bar{\nu}(\omega_0/c)^3$ (system)

(2) $\dfrac{\tau_{\rm S}^{-1}}{\tau_{\rm B}^{-1}} \propto \dfrac{\nu(\omega_0/c)^3}{\mu(\omega)} \sim \dfrac{\omega_0^3 a_0^2 V^{1/3}}{c^3} \ll 1$ or $\tau_{\rm S} \gg \tau_{\rm B} \gg \omega_0^{-1}$

8. High-dimensinal Ornstein-Ulenbeck problem for $\mathbf{q} = (x, y, x_1, y_1, x_2, y_2, \cdots)^{\mathrm{t}}$

$$\dot{P}(\mathbf{q}, t) = -\nabla \cdot [-\mathsf{F} \cdot \mathbf{q} - \mathsf{D} \cdot \nabla] \, P(\mathbf{q}, t)$$

$$\mathsf{F} = \begin{pmatrix} 0 & -\omega_0 & 0 & 0 & 0 & 0 & \cdots \\ \omega_0 & 0 & 0 & d_1 & 0 & d_2 & \cdots \\ -d_1 & 0 & \frac{\mu_1}{2} & -\omega_1 & 0 & 0 & \cdots \\ 0 & 0 & \omega_1 & \frac{\mu_1}{2} & 0 & 0 & \cdots \\ -d_2 & 0 & 0 & 0 & \frac{\mu_2}{2} & -\omega_2 & \cdots \\ 0 & 0 & 0 & 0 & \omega_2 & \frac{\mu_2}{2} & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix} = \begin{pmatrix} \mathsf{F}_S & \mathsf{F}_{\mathrm{off}} \\ \tilde{\mathsf{F}}_{\mathrm{off}} & \mathsf{F}_B \end{pmatrix}$$

$$\mathsf{D} = \begin{pmatrix} 0 & 0 & \frac{\gamma_1}{8} & 0 & \frac{\gamma_2}{8} & 0 & \cdots \\ 0 & 0 & 0 & -\frac{\gamma_1}{8} & 0 & -\frac{\gamma_2}{8} & \cdots \\ \frac{\gamma_1}{8} & 0 & \frac{\mu_1 N_1}{4} & 0 & 0 & 0 & \cdots \\ 0 & -\frac{\gamma_1}{8} & 0 & \frac{\mu_1 N_1}{4} & 0 & 0 & \cdots \\ \frac{\gamma_2}{8} & 0 & 0 & 0 & \frac{\mu_2 N_2}{2} & 0 & \cdots \\ 0 & -\frac{\gamma_2}{8} & 0 & 0 & 0 & \frac{\mu_2 N_1}{4} & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix} = \begin{pmatrix} 0 & \mathsf{D}_{\mathrm{off}} \\ \mathsf{D}_{\mathrm{off}}^{\mathrm{t}} & \mathsf{D}_B \end{pmatrix}$$

IV. Marginalization

1. Conjecture

Conditional distribution $\propto \exp\left[-\frac{1}{2}(\mathbf{q}-e^{-\mathsf{F}t}\mathbf{q}_0)^{\mathrm{t}}\cdot\mathsf{A}(t)\cdot(\mathbf{q}-e^{-\mathsf{F}t}\mathbf{q}_0)\right]$

for $\mathbf{q}=(\mathbf{r},\mathbf{R})^{\mathrm{t}}$ and initial state $\mathbf{q}_0=(\mathbf{r}_0,\mathbf{R}_0)^{\mathrm{t}}$

Conjecture based on the assumption:

– Bath quickly reaches a local equilibrium; $\tau_B \ll \tau_S$

$$P_{SB}(\mathbf{r},\mathbf{R},t|\mathbf{r}_0,0)\propto\exp\left[-\frac{1}{2}(\mathbf{R}^{\mathrm{t}}-\mathbf{u}^{\mathrm{t}})\cdot(\mathsf{A}_B+\Gamma)\cdot(\mathbf{R}-\mathbf{u})\right]P_{\mathrm{S}}(\mathbf{r},t|\mathbf{r}_0,0)$$

$$\mathsf{A}_{\mathrm{B}}=\begin{pmatrix} 2/N_1 & 0 & 0 & 0 & \cdots \\ 0 & 2/N_1 & 0 & 0 & \cdots \\ 0 & 0 & 2/N_2 & 0 & \cdots \\ 0 & 0 & 0 & 2/N_2 & \cdots \\ 0 & 0 & 0 & 0 & 2/N_3 \end{pmatrix}$$

Bare equilibrium
in the absence of interaction

– The local equilibrium is at $\mathbf{R}=\mathbf{u}(\mathbf{r},\mathbf{r}_0)$, which varies slowly in rates τ_S^{-1}.

– Not depedent on $\mathbf{R}_0$, as the initial memory decays away.

– Treat $\mathbf{u}\sim\mathcal{O}(\bar{\gamma}_i)$, $\Gamma\sim\mathcal{O}(\bar{\gamma}_i^2)$

Insight from the previous study on overdamped limit (A. Ping and C. Kwon, Complexity)

$$P(\mathbf{p},\mathbf{r},t) \propto \exp\left[-\frac{\beta}{2m}(\mathbf{p}-m\mathbf{u})^t \cdot (\mathsf{I}+\Gamma)\cdot(\mathbf{p}-m\mathbf{u}) - \phi(\mathbf{r})\right] \quad \text{for small } m/\gamma$$

$$\int d\mathbf{p} P(\mathbf{p},\mathbf{r},t)\rangle = p(\mathbf{r},t) \propto e^{-\phi}$$

$$\dot{p}(\mathbf{r},t) = -\partial_{\mathbf{r}} \cdot \mathbf{u}$$

$$\mathbf{u} = [\mathbf{f} - \mathsf{D}\cdot\partial_{\mathbf{r}}]\, p(\mathbf{r},t) \qquad \text{found self-consistently}$$

2. Substitute the conjectured $P_{\mathrm{S}}(\mathbf{r},\mathbf{R},t|\mathbf{r}_0,0)$ **to sFP equation**

$$\mathrm{LHS} = [\mathrm{Tr}\mathsf{U}_B^{-1}\dot{\Gamma}/2 + \dot{P}_{\mathrm{S}}/P_{\mathrm{S}} + \dot{\mathbf{u}}\cdot\widetilde{U}_{\mathrm{B}}\cdot\widetilde{\mathbf{R}} - \widetilde{\mathbf{R}}\cdot\dot{\Gamma}\cdot\widetilde{\mathbf{R}}/2]P$$

$$\mathrm{RHS} = [C + K_0(\mathbf{r},\mathbf{r}_0) + K_1(\widetilde{\mathbf{R}}) + K_2(\widetilde{\mathbf{R}})]P$$

$$\text{where } \widetilde{\mathbf{R}} = \mathbf{R} - \mathbf{u}$$

$$\mathsf{F} = \begin{pmatrix} \mathsf{F}_{\rm S} & \mathsf{F}_{\rm off} \\ \widetilde{\mathsf{F}}_{\rm off} & \mathsf{F}_{\rm B} \end{pmatrix} \qquad \mathsf{D} = \begin{pmatrix} 0 & \mathsf{D}_{\rm off} \\ \mathsf{D}^t_{\rm off} & \mathsf{F}_{\rm B} \end{pmatrix}$$

(i) $\dot{P}_{\rm S}/P_{\rm S} = K_0(\mathbf{r}_0)$

$$\dot{P}_S = \partial_{\mathbf{r}} \cdot (\mathsf{F}_{\rm S} \cdot \mathbf{r} + \mathsf{F}_{\rm off} \cdot \mathbf{u})\, P_S$$

(ii) $\dot{\mathbf{u}} \cdot \widetilde{U}_{\rm B} \cdot \widetilde{\mathbf{R}} = K_1(\mathbf{r}_0, \widetilde{\mathbf{R}})$

$$\dot{\mathbf{u}} = -\mathsf{F}_{\rm B} \cdot \mathbf{u} + \mathbf{r}^{\rm t} \cdot \mathsf{F}^{\rm t}_{\rm S} \cdot \partial_{\mathbf{r}} \mathbf{u} - \widetilde{\mathsf{F}}_{\rm off} \cdot \mathbf{r} + (\mathsf{F}^{\rm t}_{\rm off} - 2\mathsf{U}_{\rm B}\mathsf{D}^{\rm t}_{\rm off}) \cdot \partial_{\mathbf{r}} \ln P_{\rm S} \qquad \text{up to } \mathcal{O}(\bar{\gamma}_i)$$

(iii) $-\widetilde{\mathbf{R}} \cdot \dot{\Gamma} \cdot \widetilde{\mathbf{R}}/2 = \widetilde{\mathbf{R}}^{\rm t} \cdot \mathsf{K}_2 \cdot \widetilde{\mathbf{R}}$

$$\text{where} \quad \mathsf{K}_2 = -\Gamma \mathsf{Q}_{\rm B} \mathsf{U}_{\rm B} + \mathsf{U}_{\rm B} \mathsf{D}_{\rm B} \Gamma + (\mathsf{F}^{\rm t}_{\rm off} - 2\mathsf{U}_{\rm B}\mathsf{D}^{\rm t}_{\rm off}) \cdot \partial_{\mathbf{r}_0} \mathbf{u}$$

$$\dot{\Gamma} = -\mathsf{K}_2 - \mathsf{K}_2^{\rm t} \qquad (\text{Not needed for marginal } P_S.)$$

3. Marginal equation for system with constraint

Averaging out $\widetilde{\mathbf{R}}$ $\quad \dot{P}_{\rm S}(\mathbf{r}, t|\mathbf{r}_0, 0) = \partial_{\mathbf{r}} \cdot (\mathsf{F}_{\rm S} \cdot \mathbf{r} + \mathsf{F}_{\rm off} \cdot \mathbf{u})\, P_{\rm S}(\mathbf{r}, t|\mathbf{r}_0, 0)$

with the constraint equation

$$\dot{\mathbf{u}} = -\mathsf{F}_{\rm B} \cdot \mathbf{u} + \mathbf{r}^{\rm t} \cdot \mathsf{F}^{\rm t}_{\rm S} \cdot \partial_{\mathbf{r}} \mathbf{u} - \widetilde{\mathsf{F}}_{\rm off} \cdot \mathbf{r} + (\mathsf{F}^{\rm t}_{\rm off} - 2\mathsf{U}_{\rm B}\mathsf{D}^{\rm t}_{\rm off}) \cdot \partial_{\mathbf{r}} \ln P_{\rm S}$$

4. Additional conjecture :

$$\text{(i)}\ P_{\mathrm{S}}(\mathbf{r},t|\mathbf{r}_0,0)=\frac{[\det \mathsf{A}(t)]^{1/2}}{2\pi}\exp\left[-\frac{1}{2}(\mathbf{r}-e^{-\mathsf{F}_{\mathrm{eff}}t}\cdot\mathbf{r}_0)^{\mathrm{t}}\cdot\mathsf{A}(t)\cdot(\mathbf{r}-e^{-\mathsf{F}_{\mathrm{eff}}t}\cdot\mathbf{r}_0)\right]$$

$$\text{with the initial condition } \mathsf{A}^{-1}(0)=0$$

$$\rightarrow\quad P_{\mathrm{S}}(\mathbf{r},0|\mathbf{r}_0,0)=\delta(\mathbf{r}-\mathbf{r}_0)$$

$$\text{(ii)}\ \mathbf{u}\ \text{is linear in}\ \mathbf{r},\ \mathbf{r}_0\text{:}$$

$$\mathbf{u}=\mathsf{A}_{\mathrm{off}}\cdot\mathbf{r}+\mathsf{B}_{\mathrm{off}}e^{-\mathsf{F}_{\mathrm{eff}}t}\cdot\mathbf{r}_0$$

5. Final marginalization

$$\text{From}\quad \dot{P}_{\mathrm{S}}(\mathbf{r},t|\mathbf{r}_0,0)=\partial_{\mathbf{r}}\cdot(\mathsf{F}_{\mathrm{S}}\cdot\mathbf{r}+\mathsf{F}_{\mathrm{off}}\cdot\mathbf{u})\,P_{\mathrm{S}}(\mathbf{r},t|\mathbf{r}_0,0)$$

$$(1)\quad \mathsf{F}_{\mathrm{eff}}=\mathsf{F}_{\mathrm{S}}+\mathsf{F}_{\mathrm{off}}(\mathsf{A}_{\mathrm{off}}+\mathsf{B}_{\mathrm{off}})$$

$$(2)\quad \dot{\mathsf{A}}=\mathsf{A}(\mathsf{F}_{\mathrm{S}}+\mathsf{F}_{\mathrm{off}}\mathsf{A}_{\mathrm{off}})+(-\mathsf{F}_{\mathrm{S}}+\mathsf{A}_{\mathrm{off}}^{\mathrm{t}}\mathsf{F}_{\mathrm{off}}^{\mathrm{t}})\mathsf{A}$$

$$\text{From}\quad \dot{\mathbf{u}}=-\mathsf{F}_{\mathrm{B}}\cdot\mathbf{u}+\mathbf{r}^{\mathrm{t}}\cdot\mathsf{F}_{\mathrm{S}}^{\mathrm{t}}\cdot\partial_{\mathbf{r}}\mathbf{u}-\widetilde{\mathsf{F}}_{\mathrm{off}}\cdot\mathbf{r}+\underbrace{(\mathsf{F}_{\mathrm{off}}^{\mathrm{t}}-2\mathsf{U}_{\mathrm{B}}\mathsf{D}_{\mathrm{off}}^{\mathrm{t}})}_{\widetilde{\mathsf{D}}}\cdot\partial_{\mathbf{r}}\ln P_{\mathrm{S}}$$

$$(3)\quad \dot{\mathsf{A}}_{\mathrm{off}}=-\mathsf{F}_{\mathrm{B}}\mathsf{A}_{\mathrm{off}}+\mathsf{A}_{\mathrm{off}}\mathsf{F}_{\mathrm{S}}-\widetilde{\mathsf{F}}_{\mathrm{off}}-\widetilde{\mathsf{D}}\mathsf{A}(t)$$

$$(4)\quad \dot{\mathsf{B}}_{\mathrm{off}}=-\mathsf{F}_{\mathrm{B}}\mathsf{B}_{\mathrm{off}}+\mathsf{B}_{\mathrm{off}}\mathsf{F}_{\mathrm{eff}}+\widetilde{\mathsf{D}}\mathsf{A}(t)$$

Solving $\mathsf{A}_{\rm off}$ and $\mathsf{B}_{\rm off}$

$$(5)\quad \mathsf{A}_{\rm off}+\mathsf{B}_{\rm off}=-\int_0^t dt' e^{-\mathsf{F}_{\rm B}t'}\widetilde{\mathsf{F}}_{\rm off}e^{\mathsf{F}_{\rm S}t'}=-\mathsf{I}_1$$

$$(6)\quad \mathsf{B}_{\rm off}=\int_0^t dt'\ \underbrace{e^{-\mathsf{F}_{\rm B}t'}}_{\text{fast decaying}}\ \widetilde{\mathsf{D}}\ \underbrace{\mathsf{A}(t-t')}_{\substack{e^{\mathsf{F}_{\rm S}t'}\mathsf{A}(t)e^{-\mathsf{F}_{\rm S}t'}\\ \text{for } t\gg t'}}\ e^{\mathsf{F}_{\rm S}t'}=\int_0^t dt' e^{-\mathsf{F}_{\rm B}t'}\widetilde{\mathsf{D}}e^{\mathsf{F}_{\rm s}t'}\mathsf{A}(t)=\mathsf{I}_2\mathsf{A}(t)$$

Integrating $\mathsf{I}_{1,2}$ by parts and neglecting $e^{-\mathsf{F}_{\rm B}t}$

$$(7)\quad \mathsf{F}_{\rm B}\mathsf{I}_1-\mathsf{I}_1\mathsf{F}_{\rm S}=\widetilde{\mathsf{F}}_{\rm off}\quad\longleftarrow\quad \mathsf{I}_1=-\mathsf{F}_B^{-1}\left(e^{-\mathsf{F}_{\rm B}t'}\tilde{\mathsf{F}}_{\rm off}e^{\mathsf{F}_{\rm S}t'}\Big|_0^t-\mathsf{I}_1\mathsf{F}_{\rm S}\right)$$

$$(8)\quad \mathsf{F}_{\rm B}\mathsf{I}_2-\mathsf{I}_2\mathsf{F}_{\rm S}=\widetilde{\mathsf{D}}\ .$$

Marginal FP equation given $\mathsf{I}_{1,2}$

$$(9)\quad \dot{P}_S=\partial_{\mathbf{r}}\cdot\Big[\underbrace{\{\mathsf{F}_{\rm S}+\mathsf{F}_{\rm off}(\mathsf{A}_{\rm off}+\mathsf{B}_{\rm off})\}}_{\mathsf{F}_{\rm eff}}\cdot\mathbf{r}+\underbrace{\mathsf{F}_{\rm off}\mathsf{B}_{\rm off}\mathsf{A}(t)^{-1}}_{\mathsf{F}_{\rm off}\mathsf{I}_2,\ \text{diffusion matrix}}\partial_{\mathbf{r}}\Big]P_{\rm S}$$

$$=\partial_{\mathbf{r}}\cdot\left(\mathsf{F}_{\rm eff}\cdot\mathbf{r}+\mathsf{D}_{\rm eff}\cdot\partial_{\mathbf{r}}\right]P_{\rm S}\ .$$

where $(10)\quad \mathsf{F}_{\rm eff}=\mathsf{F}_{\rm S}-\mathsf{F}_{\rm off}\mathsf{I}_1$

$$(11)\quad \mathsf{D}_{\rm eff}=\frac{\mathsf{F}_{\rm off}\mathsf{I}_2+\mathsf{I}_2^{\rm t}\mathsf{F}_{\rm off}^{\rm t}}{2}\qquad\text{(symmetric part)}$$

V. Dynamics and steady state

1. Matrix elements of $\mathsf{F}_{\rm eff}, \mathsf{D}_{\rm eff}$

$$\sum_i \bar{\gamma}_i^2 \times g_i = \frac{\pi\nu}{V} \times \underbrace{\sum_i (e_i^x)^2 \bar{\omega}_i g_i}_{\frac{V}{(2\pi)^3}\int d^3\mathbf{k} \sum_\lambda (e^x_{\mathbf{k}\lambda})^2 (\omega/\omega_0) g(\omega/\omega_0)} = \frac{\nu(\omega_0/c)^3}{3\pi^2}\int_0^{\xi_c} d\xi\ \xi^3 g(\xi)$$

for changed variables: $k = \omega/c$, $\xi = \omega/\omega_0$, $\xi_c = \omega_c/\omega_0$

$$\mathsf{F}_{\rm eff} = \omega_0 \begin{pmatrix} 0 & -1 \\ 1+\bar{\nu} f_2 & \bar{\nu} f_1 \end{pmatrix}, \quad \mathsf{D}_{\rm eff} = \omega_0 \begin{pmatrix} 0 & \bar{\nu} d_2 \\ \bar{\nu} d_2 & \bar{\nu} 1_2 \end{pmatrix} \qquad \text{for} \quad \bar{\nu} = \nu(\omega_0/c)^3$$

Taking $\bar{\mu} \to 0$ limit and using $\dfrac{\bar{\mu}}{(\xi^2-1)^2 + \bar{\mu}^2(1+\xi^2)/2} \to \pi\delta(\xi-1)/2$

$$f_1 = \frac{1}{3\pi}\int_0^{\xi_c} d\xi\ \frac{\bar{\mu}\xi^4}{(\xi^2-1)^2 + \bar{\mu}^2(1+\xi^2)/2} \to \frac{1}{6} \qquad \text{for } \xi_c > 1$$

$$d_1 = \frac{1}{24\pi}\int_0^{\xi_c} d\xi\ \frac{\bar{\mu}\xi^3[(\xi-1)^2 + 2N(\xi)(1+\xi^2)]}{(\xi^2-1)^2 + \bar{\mu}^2(1+\xi^2)/2} \to \frac{N_0}{12} \qquad \text{for } \xi_c > 1$$

$$f_2 = -\frac{1}{3\pi}\int_0^{\xi_c} d\xi\ \frac{\xi^4(\xi^2 - 1 - \bar{\mu}^2/4)}{(\xi^2-1)^2 + \bar{\mu}^2(1+\xi^2)/2} \to -\frac{1}{3\pi}\ \mathrm{P}\int_0^{\xi_c} d\xi\ \frac{\xi^4}{\xi^2-1}$$

$$d_2 = \frac{1}{24\pi}\int_0^{\xi_c} d\xi\ \left[\frac{\xi^3(\xi^2-1)[\xi - 1 - 2N(\xi)] + \bar{\mu}^2\xi^3(1+\xi+2N(\xi))/4}{(\xi^2-1)^2 + \bar{\mu}^2(1+\xi^2)/2}\right]$$

$$\to \frac{1}{24\pi}\ \mathrm{P}\int_0^{\xi_c} d\xi\ \xi^3\left[\frac{1}{\xi+1} - \frac{2N(\xi)}{\xi^2-1}\right]$$

2. Time-dependent solution

$$P_{\mathrm{S}}(\mathbf{r},t|\mathbf{r}_0,0)=\frac{[\mathrm{detA}(t)]^{1/2}}{2\pi}\exp\left[-\frac{1}{2}(\mathbf{r}-e^{-\mathsf{F}_{\mathrm{eff}}t}\cdot\mathbf{r}_0)^{\mathrm{t}}\cdot\mathsf{A}(t)\cdot(\mathbf{r}-e^{-\mathsf{F}_{\mathrm{eff}}t}\cdot\mathbf{r}_0)\right]$$

$$P_{\mathrm{S}}(\mathbf{r},t)=\int d^2\mathbf{r}_0 P_{\mathrm{S}}(\mathbf{r},t|\mathbf{r}_0,0)P_{\mathrm{S}}(\mathbf{r}_0,0)$$

where

$$\dot{\mathsf{A}}=\mathsf{A}\mathsf{F}_{\mathrm{eff}}+\mathsf{F}_{\mathrm{eff}}^{\mathrm{t}}\mathsf{A}-2\mathsf{A}\mathsf{D}_{\mathrm{eff}}\mathsf{A}$$

$$\longrightarrow \dot{\mathsf{A}}^{-1}=-\mathsf{F}_{\mathrm{eff}}\mathsf{A}^{-1}-\mathsf{A}^{-1}\mathsf{F}_{\mathrm{eff}}^{\mathrm{t}}+2\mathsf{D}_{\mathrm{eff}} \qquad \text{using } \dot{\mathsf{A}}^{-1}=-\mathsf{A}^{-1}\dot{\mathsf{A}}\mathsf{A}^{-1}$$

$$\mathsf{A}^{-1}(t)=\mathsf{A}_{\mathrm{ss}}^{-1}-e^{-\mathsf{F}_{\mathrm{eff}}t}\mathsf{A}_{\mathrm{ss}}^{-1}e^{-\mathsf{F}_{\mathrm{eff}}^{\mathrm{t}}t} \qquad \text{where } \mathsf{A}_{ss}=\mathsf{A}(\infty)$$

3. Steady state

$$\mathsf{F}_{\mathrm{eff}}\mathsf{A}_{\mathrm{ss}}^{-1}+\mathsf{A}_{\mathrm{ss}}^{-1}\mathsf{F}_{\mathrm{eff}}^{\mathrm{t}}=2\mathsf{D}_{\mathrm{eff}}$$

$$\mathsf{A}_{\mathrm{ss}}=\begin{pmatrix}\frac{2}{N_0}+\frac{2\bar{\nu}}{N_0}\left(f_2-\frac{4}{N_0}d_2\right) & 0\\ 0 & \frac{2}{N_0}\end{pmatrix} \qquad \text{where } f_1/d_1=2/N_0$$

$$P_{\mathrm{S}}(\mathbf{r},\infty)=\frac{[\det\mathsf{A}_{\mathrm{ss}}]^{1/2}}{2\pi}\exp\left[-\frac{1}{2}\mathbf{r}^{\mathrm{t}}\cdot\mathsf{A}_{\mathrm{ss}}\cdot r\right]\to\frac{1}{\pi N_0}e^{-r^2/N_0}\ \text{as}\ \bar{\nu}\to 0$$

corresponding to $\rho_{\mathrm{S}}\propto e^{-\beta H_{\mathrm{S}}}$

4. Relaxation process governed by $e^{-\mathsf{F}_{\rm eff}t}$

Eigenvalues of $\mathsf{F}_{\rm eff}$: $\lambda_{\mp} = \omega_0\bar{\nu}f_1/2 \pm i\omega_0'$ for $\omega_0' = \omega_0(1+F_2/2)$

Relaxation rate: $\tau_{\rm S}^{-1} = \omega_0\bar{\nu}f_1 = \omega_0\dfrac{\bar{\nu}}{6} \ll \omega_0$

$$e^{-\mathsf{F}_{\rm eff}t} = e^{-t/\tau_{\rm S}}[e^{-i\omega_0't}|-\rangle\langle-| + e^{i\omega_0't}|+\rangle\langle+|]$$

where $|\pm\rangle$ ($\langle\pm|$) denotes a right (left) eigenvector of $\mathsf{F}_{\rm eff}$

$$\mathsf{A}(t) = \begin{pmatrix} \dfrac{2}{N_0\left[1-e^{-\frac{t}{\tau_{\rm S}}}\right]} + \dfrac{2F_2N_0-8D_2+e^{-\frac{t}{\tau_{\rm S}}}[4D_2-2F_2N_0]}{N_0^2\left[1-e^{-\frac{t}{\tau_{\rm S}}}\right]^2} & -\dfrac{e^{-\frac{t}{\tau_{\rm S}}}F_1N_0}{N_0^2\left[1-e^{-\frac{t}{\tau_{\rm S}}}\right]^2} \\ -\dfrac{e^{-\frac{t}{\tau_{\rm S}}}F_1N_0}{N_0^2\left[1-e^{-\frac{t}{\tau_{\rm S}}}\right]^2} & \dfrac{2}{N_0\left[1-e^{-\frac{t}{\tau_{\rm S}}}\right]} + \dfrac{e^{-\frac{t}{\tau_{\rm S}}}2D_2}{N_0^2\left[1-e^{-\frac{t}{\tau_{\rm S}}}\right]^2} \end{pmatrix}$$

$$+ \begin{pmatrix} \dfrac{e^{-\frac{t}{\tau_{\rm S}}}\left[4d_2\cos[2\omega_0't]-f_1N_0\sin[2\omega_0't]\right]}{N_0^2\left[1-e^{-\frac{t}{\tau_{\rm S}}}\right]^2} & \dfrac{e^{-\frac{t}{\tau_{\rm S}}}\left[f_1N_0\cos[2\omega_0't]+4d_2\sin[2\omega_0't]\right]}{N_0^2\left[1-e^{-\frac{t}{\tau_{\rm S}}}\right]^2} \\ \dfrac{e^{-\frac{t}{\tau_{\rm S}}}\left[f_1N_0\cos[2\omega_0't]+4d_2\sin[2\omega_0't]\right]}{N_0^2\left[1-e^{-\frac{t}{\tau_{\rm S}}}\right]^2} & \dfrac{e^{-\frac{t}{\tau_{\rm S}}}\left[2d_2\cos[2\omega_0't]+f_1N_0\sin[2\omega_0't]\right]}{N_0^2\left[1-e^{-\frac{t}{\tau_{\rm S}}}\right]^2} \end{pmatrix}.$$

5. Time evolution from initial pure state

$$\rho_S(0) = \sum_{n,m} \rho_{nm} |n\rangle\langle m|$$

$$\rightarrow P_{\rm S}(z_0, 0) = \sum_{n,m} \rho_{nm} \frac{e^{|z_0|^2}}{\sqrt{n!m!}} \frac{\partial^{n+m}}{\partial(-z_0)^n \partial(-\bar{z}_0)^m} \delta^{(2)}(z_0)$$

not positive and highly singular

A simple case: $\rho_{\rm S}(0) = |1\rangle\langle 1|$

$$P_{\rm S}(\mathbf{r}_0, 0) = e^{r_0^2} \nabla_0^2 \delta(\mathbf{r}_0)$$

$$P_{\rm S}(\mathbf{r}, t) = \frac{[{\rm detA}(t)]^{1/2}}{2\pi} \nabla_0^2 e^{r_0^2} P_{\rm S}(\mathbf{r}, t|\mathbf{r}_0, 0)\Big|_{\mathbf{r}_0=\mathbf{0}}$$

$$= \frac{[{\rm detA}(t)]^{1/2}}{8\pi} \exp\left[-\frac{1}{2}\mathbf{r}^{\rm t} \cdot {\rm A}(t) \cdot \mathbf{r}\right]$$

$$\times\Big[4 - {\rm Tr}\hat{\rm K}(t) + \left(x{\rm K}(t)_{11} + y{\rm K}(t)_{21}\right)^2 + \left(x{\rm K}(t)_{12} + y{\rm K}(t)_{22}\right)^2\Big]$$

where ${\rm K}(t) = {\rm A}(t)e^{-{\rm F}_{\rm eff}t}$, $\hat{\rm K}(t) = {}^{-{\rm F}_{\rm eff}^{\rm t}t}\ {\rm A}(t)e^{-{\rm F}_{\rm eff}t}$

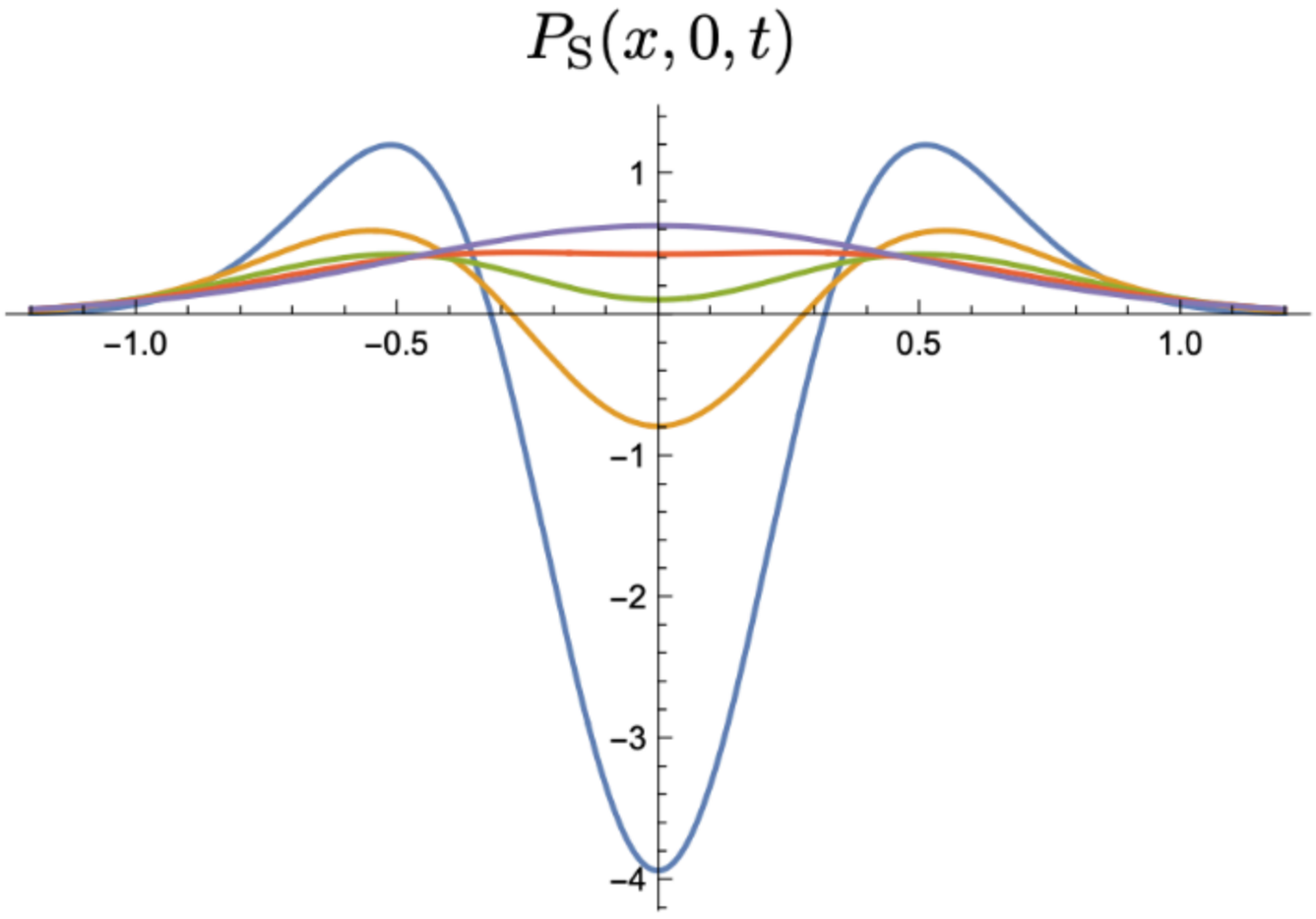


FIG. 1: $P_{\mathrm{S}}(x,0,t)$ versus x is plotted for $\bar{\nu}=0.1$, $\omega_c=2\omega_0$, and $\beta\hbar\omega_0=1$. $\tau_{\mathrm{S}}\simeq\ 592\omega_0^{-1}$. The various curves are presented for $\omega_0 t=200,\ 300,\ 400,\ 500,\ 1000$.

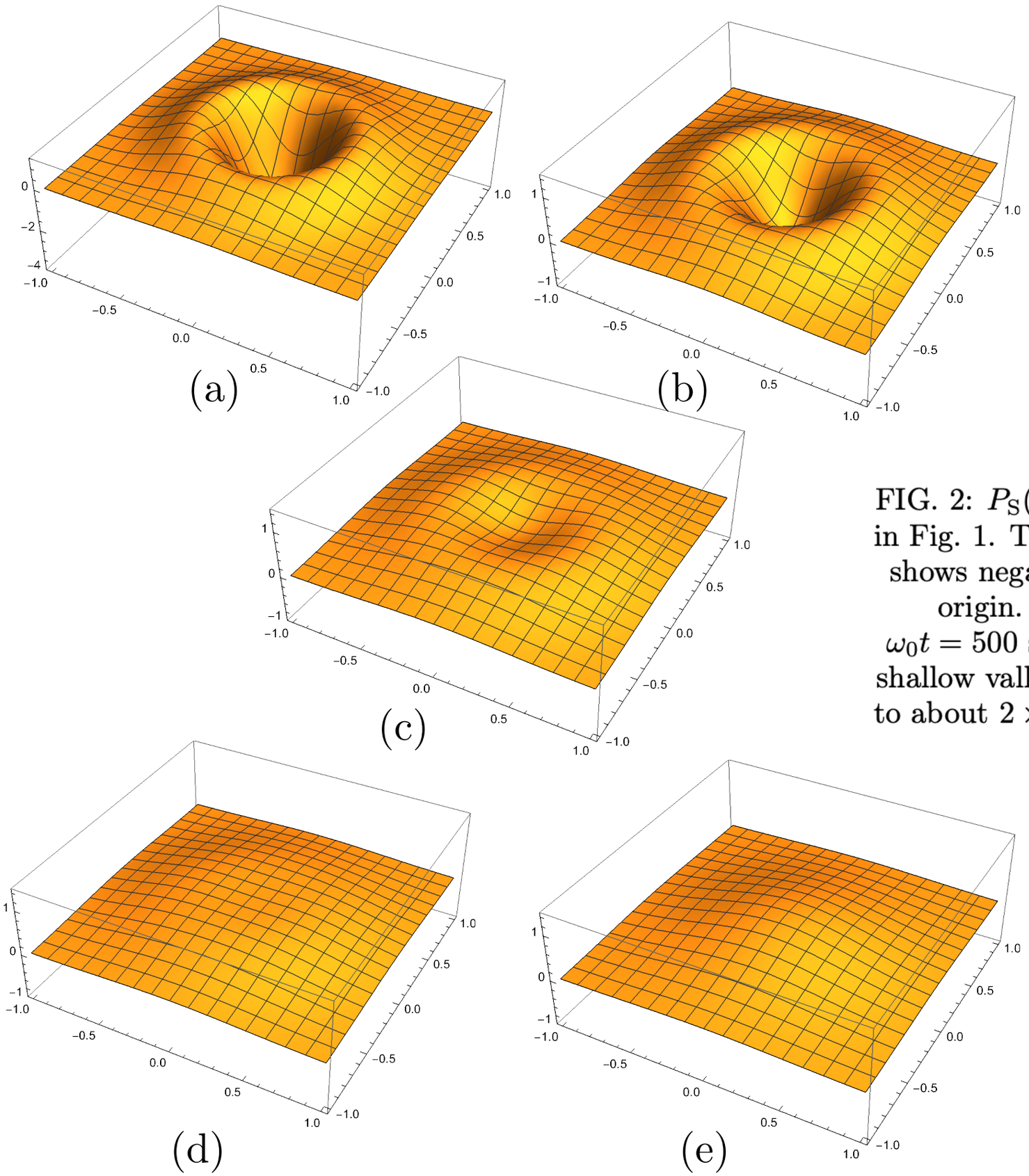


FIG. 2: $P_{\mathrm{S}}(x, y, t)$ is plotted for the same parameters as in Fig. 1. The panel (a) for $\omega_0 t = 200$, (b) for $\omega_0 t = 300$ shows negative distribution inside a valley around the origin. The panel (c) for $\omega_0 t = 400$ and (d) for $\omega_0 t = 500$ shows positive distribution everywhere with shallow valley. The panel (e) $\omega_0 t = 1000$, corresponding to about $2 \times \tau_{\mathrm{S}}$, shows distribution neary Gaussian with no valley.

VI. Steady state density matrix

Steady state P-distribution

In polar coordinates

$$P_{\rm S}^{\rm ss}=\frac{\sqrt{(2/N_0)^2(1+C\bar{\nu})}}{2\pi}\exp\left[-\frac{r^2}{N_0}(1+C\bar{\nu}\cos^2\theta)\right]$$

$$\text{where } C=f_2-\frac{4}{N_0}d_2$$

Inverse P-representation for steady state density matrix

$$\hat{\rho}_S=\int \mathrm{d}^2z|z\rangle\langle z|P_{\rm S}^{\rm ss}$$

$$=\frac{2}{N_0}\int_0^{2\pi}\frac{\mathrm{d}\theta}{2\pi}\int_0^{\infty}\mathrm{d}r e^{-\left(1+\frac{1}{N_0}\right)r^2}\sum_{m,n}\frac{|m\rangle\langle n|}{\sqrt{m!n!}}\times r^{m+n}e^{i(m-n)\theta}\left(1-\frac{C\bar{\nu}}{N_0}r^2\cos^2\theta+\frac{C\bar{\nu}}{2}\right)$$

$$=\hat{\rho}^{(0)}+\hat{\rho}^{(1)}\ .$$

$$\hat{\rho}^{(0)}=\frac{1}{N_0}\sum_{m=0}^{\infty}\frac{|m\rangle\langle m|}{(1+1/N_0)^{m+1}}=\frac{1}{Z_0}e^{-\beta\hbar\omega_0(\hat{a}^\dagger\hat{a}+1/2)}$$

$$\text{where } 1+1/N_0=e^{\beta\hbar\omega_0}$$

$$\hat{\rho}^{(1)} = \frac{2C\bar{\nu}}{N_0}\sum_m \Bigg[-\frac{1}{4N_0}\left\{ \frac{|m\rangle\langle m+2|\sqrt{(m+2)(m+1)}}{(1+1/N_0)^{m+3}} + \frac{|m\rangle\langle m-2|\sqrt{m(m-1)}}{(1+1/N_0)^{m+1}} \right\}$$

$$-\frac{1}{2}|m\rangle\langle m|\left\{ \frac{1}{N_0}\frac{m+1}{(1+1/N_0)^{m+2}} - \frac{1}{(1+1/N_0)^{m+1}} \right\}\Bigg]$$

$$= -\frac{2C\bar{\nu}}{N_0} e^{-\beta\hbar\omega_0(\hat{a}^\dagger\hat{a}+1)} \left[\frac{1}{4N_0}\left(e^{-2\beta\hbar\omega_0}\hat{a}\hat{a} + \hat{a}^\dagger\hat{a}^\dagger\right) + \frac{1}{2}\left\{ \frac{1}{N_0}e^{-\beta\hbar\omega_0}(\hat{a}^\dagger\hat{a}+1) - 1 \right\}\right]$$

$$= -\hat{\rho}^{(0)}\frac{C\bar{\nu}}{2N_0} e^{-2\beta\hbar\omega_0}\left(\hat{a}\hat{a} + e^{2\beta\hbar\omega_0}\hat{a}^\dagger\hat{a}^\dagger + 2e^{\beta\hbar\omega_0}\hat{a}^\dagger\hat{a} - 2N_0 e^{2\beta\hbar\omega_0}\right)$$

VII. Comparison with Redfield equation

Redfield equation from previous weak coupling theory

$$\dot{\rho}_S = -i[\omega_0 a^\dagger a + H_{LS}, \rho_S] + (\mathcal{L}_1 + \mathcal{L}_2)[\rho_S]$$

where

$$H_{LS} = \frac{\omega_0}{3\pi} S_+ \left(a^\dagger a + \frac{1}{2}(aa + a^\dagger a^\dagger) \right)$$

$$\mathcal{L}_1 = \frac{2\omega_0}{3}\bar{\nu}\Bigg[(N_0{+}1)\left(a\rho_S a^\dagger - \frac{1}{2}\{a^\dagger a, \rho_S\} + \frac{1}{2}\left(a\rho_S a + a^\dagger \rho_S a^\dagger - aa\rho_S - \rho_S a^\dagger a^\dagger \right) \right)$$
$$+ N_0 \left(a^\dagger \rho_S a - \frac{1}{2}\{aa^\dagger, \rho_S\} + \frac{1}{2}\left(a^\dagger \rho_S a^\dagger + a\rho_S a - a^\dagger a^\dagger \rho_S - \rho_S aa \right) \right) \Bigg]$$

$$\mathcal{L}_2 = i\frac{\omega_0}{3\pi}\bar{\nu} S_- \left(a\rho_S a - a^\dagger \rho_S a^\dagger - \frac{1}{2}\{aa - a^\dagger a^\dagger, \rho_S\} \right)$$

where

$$S_+ = \mathrm{P}\int \mathrm{d}\xi \frac{2\xi^4}{1-\xi^2} \qquad S_- = \mathrm{P}\int \mathrm{d}\xi \frac{2\xi^3(2N(\xi)+1)}{1-\xi^2}$$

P-representation

$$\dot{P}_S^{\mathrm{RF}} = \partial_{\mathbf{r}} \cdot (\mathsf{F}_{\mathrm{RF}} \cdot \mathbf{r} + \mathsf{D}_{\mathrm{RF}} \cdot \partial_{\mathbf{r}})\, P_S^{\mathrm{RF}}$$

where

$$\mathsf{F}_{\mathrm{RF}} = \omega_0 \begin{pmatrix} 0 & -1 \\ 1+\bar{\nu} f_2^{\mathrm{RF}} & \bar{\nu} f_1^{\mathrm{RF}} \end{pmatrix}, \quad \mathsf{D}_{\mathrm{RF}} = \omega_0 \begin{pmatrix} 0 & \bar{\nu} d_2^{\mathrm{RF}} \\ \bar{\nu} d_2^{\mathrm{RF}} & \bar{\nu} d_1^{\mathrm{RF}} \end{pmatrix}.$$

cf. Lindblad equation:

$$\mathsf{F}_{\mathrm{LB}} = \omega_0 \begin{pmatrix} \bar{\nu} f_1^{\mathrm{RF}}/2 & -1 \\ 1 & \bar{\nu} f_1^{\mathrm{RF}}/2 \end{pmatrix}, \quad \mathsf{D}_{\mathrm{LB}} = \omega_0 \begin{pmatrix} \bar{\nu} d_2^{\mathrm{RF}}/2 & 0 \\ 0 & \bar{\nu} d_1^{\mathrm{RF}}/2 \end{pmatrix}.$$

Comparison with our result

$$\dot{P}_S = \partial_{\mathbf{r}} \cdot (\mathsf{F}_{\mathrm{eff}} \cdot \mathbf{r} + \mathsf{D}_{\mathrm{eff}} \cdot \partial_{\mathbf{r}})\, P_S \qquad \text{Redfield-form!}$$

$$\mathsf{F}_{\mathrm{eff}} = \omega_0 \begin{pmatrix} 0 & -1 \\ 1+\bar{\nu} f_2 & \bar{\nu} f_1 \end{pmatrix}, \quad \mathsf{D}_{\mathrm{eff}} = \omega_0 \begin{pmatrix} 0 & \bar{\nu} d_2 \\ \bar{\nu} d_2 & \bar{\nu} d_1 \end{pmatrix}.$$

(A) Lindblad-type thermostat $\mathcal{L}_{\mathrm{B}}^{\mathrm{LB}}$

Remarkably

$$f_1 = f_1^{\mathrm{RF}}/4, \quad f_2 = f_2^{\mathrm{RF}}/4, \quad d_1 = d_1^{\mathrm{RF}}/4, \quad d_2 = d_2^{\mathrm{RF}}/4$$

$\longrightarrow$ $f_1/d_1 = f_1^{\mathrm{RF}}/d_1^{\mathrm{RF}}$ equililibrium in the leading order

$C = f_2 - 4d_2/N_0 = C^{\mathrm{RF}}/4$ different correction

(B) Redfield-type thermostat $\mathcal{L}_{\rm B}^{\rm RF}$

$$\mathsf{F}_{\rm B}^{i} = \begin{pmatrix} 0 & -\omega_i \\ \omega_i + \mu_0 \omega_i Q_i & \mu_0 \omega_i J_i \end{pmatrix} \qquad \text{cf: LB-type} \quad \begin{pmatrix} \mu_0 \omega_i J_i/2 & -\omega_i \\ \omega_i & \mu_0 \omega_i J_i/2 \end{pmatrix}$$

$$\text{where} \qquad J_i = J(\omega_i)\ , \qquad Q_i \propto \mathrm{P}\int_0^{\omega_c} \mathrm{d}\Omega \frac{\Omega^2 J(\Omega)}{\Omega^2 - \omega_i^2} \quad ,\ \mu_0 \sim V^{-1/3}$$

$$f_1 = \alpha f_1^{\rm RF}, \quad f_2 = f_2^{\rm RF}/4, \quad d_1 = \alpha d_1^{\rm RF}, \quad d_2 = d_2^{\rm RF}/4$$

Only diagonal elements are changed.

$$\text{with} \quad \alpha = \frac{J_0}{4\sqrt{J_0^2 + Q_0^2}}$$

General type

$$\mathsf{F}_{\mathrm{B}}^{i} = \begin{pmatrix} \mu_0 \tilde{p}_i & -\omega_i \\ \omega_i + \mu_0 q_i & \mu_0 p_i \end{pmatrix} \qquad \alpha = \frac{1}{4} \frac{p_0 + \tilde{p}_0}{\sqrt{q_0^2 + (p_0 + \tilde{p}_0)^2}}$$

LB-type: $p_0 = \tilde{p}_0$, $q_0 = 0$, $\alpha = 1/4$

RF-type: $\tilde{p}_0 = 0$, $q_0 \neq 0$, $\alpha = \dfrac{p_0}{4\sqrt{q_0^2 + p_0^2}}$

Fixed $f_1/d_1 = 2/N_0$, $C = f_2 - 4d_2/N_0$

– Steady state is independent of thermostat (dissipator of B).

VIII. About mean-force-Gibbs

From Thinga, Wang, Hänggi, JCP, (2012); Lee and Yeo, PRE (2022)

$$\hat{\rho}_{\rm MFG} = {\rm Tr}_B e^{-\beta(H_S+H_B+H_I)} \simeq \hat{\rho}^{(0)} \left(\mathsf{I} - \epsilon^2(\mathsf{D}_{\rm off} + \mathsf{D}_{\rm diag})\right)$$

$$\text{where } \hat{\rho}^{(0)} = e^{-\beta H_S}/Z_0$$

(1) $\mathsf{D}_{\rm off}$ is equal to that from the Redfield equation.

(2) $\mathsf{D}_{\rm diag}$ is equal to that obtained by a special analytic continuation from $\mathsf{D}_{\rm off}$.

Our claim:

– $\mathsf{D}_{\rm diag}$ is *not equal* to that obtained by standard perturbation expansion for the Redfield equation. In our case

$$\hat{\rho}^{(0)}\mathsf{D}_{\rm diag} \neq \hat{\rho}^{(0)} \frac{C_{\rm RF}\bar{\nu}}{2N_0} e^{-2\beta\hbar\omega_0} \left(2e^{\beta\hbar\omega_0}\hat{a}^\dagger\hat{a} - 2N_0 e^{2\beta\hbar\omega_0}\right)$$

$$\text{where } C_{\rm RF} = f_2^{\rm RF} - 4d_2^{\rm RF}/N_0$$

– The Redfield equation is not a rigorous result from the unitary dynamics:

$$\dot{\hat{\rho}} = -i[H_S + H_B + H_I, \hat{\rho}]$$

So, the steady state of the Redfield equation may not be MFG.

– The steady state of our dynamics is definitely not MFG and can provide an expectation for real experiments performed for baths open to environment.

IX. Discussions

1. We investigated thermodynamics of a small quantum system coupled with a dissipative (thermostatted) bath by introducing a super bath maintained at fixed temperature.

2. Our perspective on system and bath open to outer environment is more realistic than the previous weak coupling theory.

3. Independent of thermostat (type of dissipator of bath), the reduced (marginal) dynamics of the system has the same form as the Redfield dynamics with different coefficients. The derived steady state is independent of thermostat, while dynamics depends on it. It might well describe that the steady state of the system, especially the deviation from Boltzmann state, depends on the interaction and temperature of bath while the system's dynamics depends on a kind of environment open to the bath since it has a strong influence on the bath's dynamics.

4. Our approach fully takes dissipative nature of bath into account; for example we find $\mathbf{u}$ as a measure of correlation between the system and bath, which is not possible from the conventional Redfield equation.

5. The steady state from our theory, that is definitely not equal to the MFG state, may provide a realistic expectation.

6. We will extend our approach to general non-harmonic cases such as a two-level system.

7. We can study nonequilibrium thermodynmics for time dependent Hamiltonian systems, that cannot be handled rigorously in the Redfield or Lindblad equation.