Multimode Brownian oscillators: Thermodynamics and heat transport

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In this work, we investigate the multimode Brownian oscillators in nonequilibrium scenarios with multiple reservoirs at different temperatures. For this purpose, an algebraic method is proposed. This approach directly gives the exact time–local equation of motion for reduced density operator, from which we can easily extract both the reduced system and hybrid bath dynamical informations. Two representative entangled system–bath quantities, the heat transport and the thermodynamics of quantum mixing, are studied. The heat current is obtained from both the algebraic method and the discrete imaginary–frequency method followed by the Meir–Wingreen's formula. It is anticipated that the algebraic method developed in this work would constitute a crucial component for nonequilibrium statistical mechanics for open quantum systems.

I. INTRODUCTION

Open quantum systems play pivotal roles in diversed fields such as nuclear magnetic resonance,[1–3] condensed matter and material physics,[4–6] high energy physics,[7–9] quantum optics,[10–12] chemical and biological physics,[13–15] and nonlinear spectroscopy.[16–20] In most of these studies, the system and its environment constitute a thermodynamic composite. Thermal effects dictate the system–environment entanglement, which is intimately related to the thermodynamic and transport properties.[21–28] Practically, these properties are under focus in manipulating mesoscopic nanodevices.[29–33]

Among them, the real-time evolution of heavy quarkonium in the quark-gluon plasma was investigated by Miura *et.al*[9] by means of open quantum system theory. Their results provided novel comprehension on mechanism of dynamics of the relative motion of the quarkonium state over time influenced by quantum dissipation. When considering a point charge emitting radiation in an electromagnetic field, Hsiang *et.al*[34] pointed out the internal degrees of freedom of a moving atom can be modeled by a harmonic oscillator coupled to a scalar field. Following the same coupling ways as scalar electrodynamics, the pathologies of radiation reaction can be recast as non-Markovian dynamics of a Brownian oscillator in a supra-Ohmic environment. In terms of quantum decoherence and measurement, Anglin[35] *et.al* introduced Brownian harmonic oscillator as one of their toy models to study universalities in the phenomenology of decoherence. An easy derivation of the short-time behavior of the Wigner function for an Ohmic Brownian oscillator was also given by them. All of their results introduced or did researches on Brownian oscillator (BO). The significance of this model can be never underestimated.

As a typical open quantum system, the BO is the simplest and exactly solvable model. It serves as an elementary example in various studies.[36–39] Among them, both application and theoretical aspects on various perturbative formulations. BO has been investigated widely in terms of real–time dynamics.[40–46]Ford[44] *et.al* obtained an exact general solution in the form of an expression for the Wigner function at time t in terms of the initial Wigner function which is later applied to the motion of a Gaussian wave packet and to that of a pair of such wave packets. In thermodynamics[47,48], Huang *et.al*[48] investigated the thermodynamic quantities of the reduced BO system, finding that the steady state can be expressed as the Gibbs state with the renormalized system Hamiltonian. Most of these studies had mainly focused on the reduced system, but not the underlying hybrid bath properties. On the other hand, we develop the free-energy spectrum theory for thermodynamics of system–bath mixing that can be either fermionic or bosonic or combined.[27]

In this work, we develop an algebraic approach to obtain the equation of motion (EOM) for the multimode BO system, from which we can easily extract both the reduced system and hybrid bath dynamical informations. Besides, as two representative entangled system–bath quantities, we exploit the well-established EOM to study the heat transport and the thermodynamics of quantum mixing. To obtain the nonequilibrium correlation functions, we also develop the discrete imaginary–frequency (DIF) method.

The remainder of this paper is organized as follows. In Sec. II we present the exact EOM of the multimode BO system via the algebraic approach. Especially, we emphasize how to extract the hybrid bath informations. Based on these formulations, in Sec. III we investigate the heat current and thermodynamics. We finally summarize this paper in Sec. V. Throughout this paper we set $\hbar = 1$ and $\beta = 1/(k_B T_\alpha)$ with k_B being the Boltzmann constant and T_α the temperature of the α-reservoir.

II. EOM FOR MULTIMODE BO SYSTEM

In this section, we present the exact EOM of the multimode BO system via the algebraic approach.

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A. EOM for coordinates and momentums

We introduce the multimode Brownian oscillator model. The total Hamiltonian reads

$$\begin{aligned}H_{\rm T} &= H_{\rm S} + H_{\rm SB} + h_{\rm B}\\ &= \sum_u \frac{\hat P_u^2}{2} + \frac{1}{2}\sum_{uv} V_{uv}\hat Q_u \hat Q_v - \sum_{\alpha u}\hat Q_u \hat F_{\alpha u} + \sum_\alpha h_\alpha^{\rm B}.\end{aligned} \tag{1}$$

Here, $\{\hat P_u\}$ and $\{\hat Q_u\}$ denote the mass–scaled momentums and coordinates of the system, respectively. The noninteracting reservoir of $h_{\rm B} = \sum_\alpha h_\alpha^{\rm B}$ together with the random forces $\{\hat F_{\alpha u}\}$ constitute a Gaussian environment. The precursor to the conventional quantum Langevin equation can be obtained from the Hamiltonian of Eq. (1) as[49–51]

$$\hat F_{\alpha u}(t) = \hat F^{\rm B}_{\alpha u}(t) + \sum_v \int_0^t {\rm d}\tau\, \phi_{\alpha uv}(t-\tau)\hat Q_v(\tau) \tag{2}$$

where $\hat F^{\rm B}_{\alpha u}(t) \equiv e^{ih^{\rm B}_\alpha t}\hat F_{\alpha u} e^{-ih^{\rm B}_\alpha t}$ and

$$\phi_{\alpha uv}(t) \equiv i\langle[\hat F^{\rm B}_{\alpha u}(t), \hat F^{\rm B}_{\alpha v}(0)]\rangle_{\rm B}. \tag{3}$$

The average is defined as $\langle(\,\cdot\,)\rangle_{\rm B} \equiv {\rm tr}_{\rm B}[(\,\cdot\,)\rho^0_{\rm B}]$ with $\rho^0_{\rm B} = \otimes_\alpha[e^{-\beta_\alpha h^{\rm B}_\alpha}/{\rm tr}_{\rm B}(e^{-\beta_\alpha h^{\rm B}_\alpha})]$. For later use, we introduce the hybrid bath correlation function

$$c_{\alpha uv}(t) \equiv \langle \hat F^{\rm B}_{\alpha u}(t)\hat F^{\rm B}_{\alpha v}(0)\rangle_{\rm B}. \tag{4}$$

Together with the time–reversal relation, we know that $\phi_{\alpha uv}(t) = i[c_{\alpha uv}(t) - c^*_{\alpha uv}(t)]$.

The time evolutions of system coordinates and moments can be resolved as[38,46]

$$\begin{bmatrix}\hat{\boldsymbol Q}(t)\\ \hat{\boldsymbol P}(t)\end{bmatrix} = \mathbf T(t)\begin{bmatrix}\hat{\boldsymbol Q}(0)\\ \hat{\boldsymbol P}(0)\end{bmatrix} + \sum_\alpha \int_0^t {\rm d}\tau\, \mathbf T(t-\tau)\begin{bmatrix}0\\ \hat{\boldsymbol F}^{\rm B}_\alpha(\tau)\end{bmatrix}. \tag{5}$$

For compactness, we have introduced vectors and matrices, $\hat{\boldsymbol P} \equiv \{\hat P_u\}$, $\hat{\boldsymbol Q} \equiv \{\hat Q_u\}$, $\hat{\boldsymbol F}^{\rm B}_\alpha \equiv \{\hat F^{\rm B}_{\alpha u}\}$, and

$$\mathbf T(t) = \begin{bmatrix} -\boldsymbol\chi_{QP}(t) & \boldsymbol\chi_{QQ}(t)\\ -\boldsymbol\chi_{PP}(t) & \boldsymbol\chi_{PQ}(t)\end{bmatrix} = \begin{bmatrix}\dot{\boldsymbol\chi}(t) & \boldsymbol\chi(t)\\ \ddot{\boldsymbol\chi}(t) & \dot{\boldsymbol\chi}(t)\end{bmatrix}. \tag{6}$$

Here,

$$\boldsymbol\chi(t) \equiv \{\chi_{uv}(t) = i\langle[Q_u(t), Q_v(0)]\rangle\} \tag{7}$$

with the average $\langle(\,\cdot\,)\rangle$ over the total composite steady state. The time–local equation of motion is then obtained from Eq. (5) as

$$\begin{bmatrix}\dot{\hat{\boldsymbol Q}}(t)\\ \dot{\hat{\boldsymbol P}}(t)\end{bmatrix} = \boldsymbol\Lambda(t)\begin{bmatrix}\hat{\boldsymbol Q}(t)\\ \hat{\boldsymbol P}(t)\end{bmatrix} + \sum_\alpha \begin{bmatrix}0\\ \hat{\boldsymbol F}^{\rm eff}_\alpha(t)\end{bmatrix}. \tag{8}$$

Here, the matirx $\boldsymbol\Lambda(t)$ is the key quantity, reading

$$\boldsymbol\Lambda(t) = \dot{\mathbf T}(t)\mathbf T^{-1}(t) \equiv \begin{bmatrix}\boldsymbol\Lambda_{QQ}(t) & \boldsymbol\Lambda_{QP}(t)\\ \boldsymbol\Lambda_{PQ}(t) & \boldsymbol\Lambda_{PP}(t)\end{bmatrix} \tag{9}$$

with

$$\boldsymbol\Lambda_{QQ}(t) = \mathbf 0, \tag{10a}$$
$$\boldsymbol\Lambda_{QP}(t) = \mathbf I, \tag{10b}$$
$$\boldsymbol\Lambda_{PQ}(t) = -\boldsymbol\Omega(t), \tag{10c}$$
$$\boldsymbol\Lambda_{PP}(t) = -\boldsymbol\Gamma(t), \tag{10d}$$

and

$$\begin{aligned}\boldsymbol F^{\rm eff}_\alpha(t) = \boldsymbol F^{\rm B}_\alpha(t) + \int_0^t {\rm d}\tau\,\big[&\boldsymbol\Omega(t)\boldsymbol\chi(t-\tau)\\ &+ \boldsymbol\Gamma(t)\dot{\boldsymbol\chi}(t-\tau) + \ddot{\boldsymbol\chi}(t-\tau)\big]\boldsymbol F^{\rm B}_\alpha(\tau).\end{aligned} \tag{11}$$

In Eqs. (10) and (11),

$$\boldsymbol\Omega = \dddot{\boldsymbol\chi}(\boldsymbol\chi\dot{\boldsymbol\chi}^{-1}\ddot{\boldsymbol\chi} - \dot{\boldsymbol\chi})^{-1} - \ddot{\boldsymbol\chi}(\boldsymbol\chi - \dot{\boldsymbol\chi}\ddot{\boldsymbol\chi}^{-1}\dot{\boldsymbol\chi})^{-1}, \tag{12a}$$
$$\boldsymbol\Gamma = \dddot{\boldsymbol\chi}(\dot{\boldsymbol\chi}\boldsymbol\chi^{-1}\dot{\boldsymbol\chi} - \ddot{\boldsymbol\chi})^{-1} - \ddot{\boldsymbol\chi}(\dot{\boldsymbol\chi} - \ddot{\boldsymbol\chi}\dot{\boldsymbol\chi}^{-1}\boldsymbol\chi)^{-1}, \tag{12b}$$

by using

$$\mathbf T^{-1}(t) = \begin{bmatrix}(\dot{\boldsymbol\chi} - \boldsymbol\chi\dot{\boldsymbol\chi}^{-1}\ddot{\boldsymbol\chi})^{-1} & (\ddot{\boldsymbol\chi} - \dot{\boldsymbol\chi}\boldsymbol\chi^{-1}\dot{\boldsymbol\chi})^{-1}\\ (\boldsymbol\chi - \dot{\boldsymbol\chi}\ddot{\boldsymbol\chi}^{-1}\dot{\boldsymbol\chi})^{-1} & (\dot{\boldsymbol\chi} - \ddot{\boldsymbol\chi}\dot{\boldsymbol\chi}^{-1}\boldsymbol\chi)^{-1}\end{bmatrix}. \tag{13}$$

Detailed derivation is given in the Sec. A of the supporting materials (SM), where we also gives EOM of first and second order moments for later use.

B. EOM for reduced density operator

By applying Liouville-von Neumann equation to the total density operater, $\dot\rho_{\rm T}(t) = -i[H_{\rm T}, \rho_{\rm T}(t)]$, we obtain for $\rho_{\rm S}(t) = {\rm tr}_{\rm B}\rho_{\rm T}(t)$ the EOM as the following:

$$\begin{aligned}\dot\rho_{\rm S}(t) = &-i\Big[\sum_u \frac{\hat P_u^2}{2} + \frac{1}{2}\sum_{uv} V_{uv}\hat Q_u\hat Q_v, \rho_{\rm S}(t)\Big]\\ &-i\sum_{\alpha u}[\hat Q_u, \varrho_{\alpha u}(t)]\end{aligned} \tag{14}$$

where

$$\varrho_{\alpha u}(t) \equiv {\rm tr}_{\rm B}[\hat F_{\alpha u}\rho_{\rm T}(t)], \tag{15}$$

named as the hybrid density operator (HDO) in this work. Because of the Gaussian property of the current BO system, $\varrho_{\alpha u}$ is of the form

$$\varrho_{\alpha u}(t) \equiv \sum_v \big[\varrho^{(1)}_{\alpha uv}(t) + \varrho^{(2)}_{\alpha uv}(t)\big], \tag{16}$$

where

$$\varrho^{(1)}_{\alpha uv}(t) = \big[\Omega_{\alpha uv}(t)\hat Q^{\oplus}_v + \Gamma_{\alpha uv}(t)\hat P^{\oplus}_v\big]\rho_{\rm S}(t), \tag{17a}$$
$$\varrho^{(2)}_{\alpha uv}(t) = \big[\gamma_{\alpha uv}(t)\hat Q^{\ominus}_v - \gamma'_{\alpha uv}(t)\hat P^{\ominus}_v\big]\rho_{\rm S}(t), \tag{17b}$$

with

$$A^{\oplus}\hat O \equiv \frac{1}{2}\{\hat A, \hat O\} \quad \text{and} \quad A^{\ominus}\hat O \equiv -i[\hat A, \hat O]. \tag{18}$$

As seen in the Sec. B of SM, the time–dependent coefficients in Eq. (17a) can be obtained from the centers of phase–space wavepacket, whereas those in Eq. (17b) be from the variances. Here, we summarize the final results, reading

$$\begin{bmatrix}\boldsymbol{\Omega}_\alpha(t)\\ \boldsymbol{\Gamma}_\alpha(t)\end{bmatrix}^T = -\int_0^t \mathrm{d}\tau \begin{bmatrix}\boldsymbol{\phi}_\alpha(t-\tau)\\ 0\end{bmatrix}^T \mathbf{T}(\tau)\mathbf{T}^{-1}(t), \quad (19)$$

and

$$\begin{bmatrix}\boldsymbol{\gamma}'_\alpha(t) & \boldsymbol{\gamma}_\alpha(t)\end{bmatrix} = \begin{bmatrix}\boldsymbol{\Omega}(t) & \boldsymbol{\Gamma}(t) & \mathbf{I}\end{bmatrix} \begin{bmatrix}[\boldsymbol{k}^{00}_\alpha(t)]^{\mathrm{T}} & [\boldsymbol{k}^{10}_\alpha(t)]^{\mathrm{T}}\\ [\boldsymbol{k}^{01}_\alpha(t)]^{\mathrm{T}} & [\boldsymbol{k}^{11}_\alpha(t)]^{\mathrm{T}}\\ [\boldsymbol{k}^{02}_\alpha(t)]^{\mathrm{T}} & [\boldsymbol{k}^{12}_\alpha(t)]^{\mathrm{T}}\end{bmatrix} \quad (20)$$

where

$$\boldsymbol{u}_\alpha(t) \equiv \int_0^t \mathrm{d}\tau\, \boldsymbol{\chi}(t-\tau)\mathrm{Re}\boldsymbol{c}_\alpha(\tau), \quad (21a)$$

$$\boldsymbol{k}^{ij}_\alpha(t) = \int_0^t \mathrm{d}\tau \left[\mathcal{D}_i\boldsymbol{\chi}(\tau)\mathcal{D}_j\boldsymbol{u}^{\mathrm{T}}_\alpha(\tau) + \mathcal{D}_i\boldsymbol{u}_\alpha(\tau)\mathcal{D}_j\boldsymbol{\chi}^{\mathrm{T}}(\tau)\right], \quad (21b)$$

with and a notation for derivative operator as $\mathcal{D}_m \to d^m/d\tau^m$. Detailed derivations are given in the SM.

C. Analysis at $t = 0$

Emerged in the time–local EOM Eq. (8) below will will be the time–local frequency and friction functions, $\boldsymbol{\Omega}(t)$ and $\boldsymbol{\Gamma}(t)$, defined via the transfer matrix, Eq. (9) and Eq. (10). And we have their explicit expression as Eq. (12). The initial values are $\boldsymbol{\Omega}(0) = \boldsymbol{V}$ and $\boldsymbol{\Gamma}(0) = \mathbf{0}$, which agree with the general picture of non-Markovian friction that takes effects only after a certain finite time.

First of all, we can prove that

$$\boldsymbol{\Omega}(t)\boldsymbol{\chi}(t) + \boldsymbol{\Gamma}(t)\dot{\boldsymbol{\chi}}(t) = -\ddot{\boldsymbol{\chi}}(t) \quad (22a)$$

$$\boldsymbol{\Omega}(t)\dot{\boldsymbol{\chi}}(t) + \boldsymbol{\Gamma}(t)\ddot{\boldsymbol{\chi}}(t) = -\dddot{\boldsymbol{\chi}}(t) \quad (22b)$$

take the derivation of Eq. (22a) and substract Eq. (22b) from that we get

$$\dot{\boldsymbol{\Omega}}(t)\boldsymbol{\chi}(t) + \dot{\boldsymbol{\Gamma}}(t)\dot{\boldsymbol{\chi}}(t) = \mathbf{0}. \quad (23)$$

We first introduced various kinds of response functions togethered with $\chi_{uv}(t)$,

$$\chi^{\mathrm{SB}}_{\alpha uv}(t) = i\langle[\hat{Q}_u(t), \hat{F}_{\alpha v}(0)]\rangle, \quad (24)$$

$$\chi^{\mathrm{BB}}_{\alpha uv}(t) = i\langle[\hat{F}_{\alpha u}(t), \hat{F}_{\alpha v}(0)]\rangle, \quad (25)$$

for the short–time behaviors of response functions, we have the following properties,

$$\boldsymbol{\chi}(0) = \ddot{\boldsymbol{\chi}}(0) = \ddddot{\boldsymbol{\chi}}(0) = \mathbf{0}, \quad \dot{\boldsymbol{\chi}}(0) = \mathbf{I}, \quad \dddot{\boldsymbol{\chi}}(0) = -\boldsymbol{V}, \quad (26)$$

$$\boldsymbol{\chi}^{\mathrm{SB}}_\alpha(0) = \ddot{\boldsymbol{\chi}}^{\mathrm{SB}}_\alpha(0) = \dot{\boldsymbol{\chi}}^{\mathrm{SB}}_\alpha(0) = \mathbf{0}, \quad (27)$$

$$\boldsymbol{\chi}^{\mathrm{BB}}_\alpha(0) = \ddot{\boldsymbol{\chi}}^{\mathrm{BB}}_\alpha(0) = \mathbf{0}, \quad \dot{\boldsymbol{\chi}}^{\mathrm{BB}}_\alpha(0) = \dot{\boldsymbol{\phi}}_\alpha(0), \quad (28)$$

while the short–time behaviors of $\boldsymbol{\Omega}(t)$ and $\boldsymbol{\Gamma}(t)$ can then be proved to be

$$\begin{aligned}&\boldsymbol{\Omega}(0) = \boldsymbol{V}, \quad \boldsymbol{\Gamma}(0) = \dot{\boldsymbol{\Omega}}(0) = \dot{\boldsymbol{\Gamma}}(0) = \ddot{\boldsymbol{\Gamma}}(0) = \mathbf{0},\\ &\ddot{\boldsymbol{\Omega}}(t) = -\sum_\alpha \dot{\boldsymbol{\phi}}_\alpha(0), \dddot{\boldsymbol{\Gamma}}(0) = 2\sum_\alpha \dot{\boldsymbol{\phi}}_\alpha(0),\\ &\lim_{t\to 0} \dot{\boldsymbol{\Gamma}}^{-1}(t)\dot{\boldsymbol{\Omega}}(t)\boldsymbol{\chi}(t) = -\mathbf{I}. \end{aligned} \quad (29)$$

Detailed proofs and long–time behaviors of $\boldsymbol{\gamma}_\alpha(t)$ and $\boldsymbol{\gamma}'_\alpha(t)$ can be found in the SM.

III. ENTANGLED SYSTEM–BATH PROPERTIES

A. Thermodynamics free energy

Turn to the thermodynamics free–energy change before and after the system–bath mixing. Here, only the single reservoir of temperature T is involved. In the previous work, we have proven that the free–energy change can be expressed as[27]

$$\begin{aligned}A_{\mathrm{hyb}}(T) &= -\frac{1}{\pi}\int_{-\infty}^{\infty}\mathrm{d}\omega\, \frac{\varphi(\omega)}{1-e^{-\beta\omega}}\\ &= -\frac{1}{\beta}\vartheta(0) - \frac{2}{\beta}\sum_{n=1}^{\infty}\vartheta(\varpi_n), \end{aligned} \quad (30)$$

with $\{\varpi_n = 2n\pi/\beta\}$ being the bosonic Matsubara frequencies. In Eq. (30), $\varphi(\omega)$ and $\vartheta(\varpi > 0)$ are defined as

$$\varphi(\omega) = \frac{1}{2}\,\mathrm{Im}\int_0^1 \mathrm{d}\lambda^2\, \mathrm{tr}\big[\widetilde{\boldsymbol{\phi}}(\omega)\widetilde{\boldsymbol{\chi}}(\omega;\lambda)\big], \quad (31)$$

$$\vartheta(\varpi) = \frac{1}{2}\int_0^1 \mathrm{d}\lambda^2\, \mathrm{tr}\big[\widetilde{\boldsymbol{\phi}}(i\varpi)\widetilde{\boldsymbol{\chi}}(i\varpi;\lambda)\big], \quad (32)$$

where

$$\widetilde{f}(\omega) \equiv \int_0^\infty \mathrm{d}t\, e^{i\omega t} f(t) \quad (33)$$

and $\boldsymbol{\chi}(t;\lambda)$ is defined when the system–bath interaction term, H_{SB} in Eq. (1), is multiplied by a mixing parameter, $\lambda \in [0,1]$, i.e., $H_{\mathrm{SB}} \to \lambda H_{\mathrm{SB}}$. There exists the equal area relation, reading

$$\int_0^\infty \mathrm{d}\omega\, \vartheta(\omega) = \int_0^\infty \mathrm{d}\omega\, \varphi(\omega). \quad (34)$$

B. Heat transport

Consider the heat transport from the α–reservoir to the local impurity system. The heat current operator reads

$$\hat{J}_\alpha \equiv -\frac{\mathrm{d}h_\alpha}{\mathrm{d}t} = -i[H_{\mathrm{T}}, h_\alpha] = -\sum_u \hat{Q}_u \dot{\hat{F}}_{\alpha u}. \quad (35)$$

We can prove,

$$\left\langle \hat{J}_\alpha(t) \right\rangle = -\sum_u \mathrm{tr}_{\mathrm{S}} \left[\hat{Q}_u \dot{\varrho}_{\alpha u}(t) \right] + \sum_u \mathrm{tr}_{\mathrm{S}} \left[\hat{P}_u \varrho_{\alpha u}(t) \right], \tag{36}$$

Alternatively, the heat current can be recast as

$$J_\alpha = -2\,\mathrm{Im}\int_0^\infty \mathrm{d}\tau\, \mathrm{tr}\big[\dot{\boldsymbol{c}}_\alpha(\tau)\boldsymbol{C}_{\mathrm{SS}}(\tau)\big]. \tag{37}$$

This is the time–domain Meir–Wingreen's formula. In the frequency domain, it reads

$$J_\alpha = -\frac{2}{\pi}\sum_{uv}\int_{-\infty}^{\infty}\mathrm{d}\omega\, \frac{\omega}{e^{\beta_\alpha \omega}-1} J^\alpha_{uv}(\omega) C_{vu}(\omega), \tag{38}$$

where

$$J^\alpha_{uv}(\omega) \equiv \frac{1}{2i}\int_{-\infty}^{\infty}\mathrm{d}t\, e^{i\omega t}\phi_{uv}(t), \tag{39}$$

and

$$C_{uv}(\omega) \equiv \frac{1}{2}\int_{-\infty}^{\infty}\mathrm{d}t\, e^{i\omega t}\langle \hat{Q}_u(t)\hat{Q}_v(0)\rangle. \tag{40}$$

IV. NUMERICAL RESULTS

Introducing Meir–Wingreen's formula to obtain heat current needs correlation function. Therefore we develop a so–called discrete imaginary–frequency method (DIF) method to obtain correlation function of the system. Besides, entanglement spectrum is also at hand with the help of entanglement thereom.

We start from expanding $c_{\alpha uv}(t)$ as

$$c_{\alpha uv}(t) = \sum_k g_{\alpha uvk} e^{-\gamma_{\alpha k} t}, \tag{41}$$

and from which we derive the following equations

$$\tilde{\boldsymbol{C}}(\omega) = \Big[\boldsymbol{V} - \omega^2\mathbf{I} - \sum_\alpha \tilde{\phi}_\alpha(\omega)\Big]^{-1}\Big[\dot{\boldsymbol{C}}(0) - i\omega\boldsymbol{C}(0) + \sum_\alpha \tilde{\boldsymbol{X}}_\alpha(\omega)\Big] \tag{42a}$$

$$\tilde{\boldsymbol{X}}_\alpha(\omega) = -\sum_k \frac{2}{\gamma_{\alpha k} - i\omega}\,\mathrm{Im}\big[\tilde{\boldsymbol{C}}(i\gamma_{\alpha k})\boldsymbol{g}_{\alpha k}\big]^{\mathrm{T}}, \tag{42b}$$

Let $\omega = i\gamma_{\alpha' k'}$ in Eq. (42) we obtain following equations

$$\tilde{\boldsymbol{C}}(i\gamma_{\alpha' k'}) = \Big[\boldsymbol{V} + \gamma^2_{\alpha' k'}\mathbf{I} - \sum_\alpha \tilde{\phi}_\alpha(i\gamma_{\alpha' k'})\Big]^{-1}\Big[\dot{\boldsymbol{C}}(0) + \gamma_{\alpha' k'}\boldsymbol{C}(0) + \sum_\alpha \tilde{\boldsymbol{X}}_\alpha(i\gamma_{\alpha' k'})\Big] \tag{43a}$$

$$\tilde{\boldsymbol{X}}_\alpha(i\gamma_{\alpha' k'}) = -\sum_k \frac{2}{\gamma_{\alpha' k'} + \gamma_{\alpha k}}\,\mathrm{Im}\big[\tilde{\boldsymbol{C}}(i\gamma_{\alpha k})\boldsymbol{g}_{\alpha k}\big]^{\mathrm{T}}, \tag{43b}$$

from the equations above we can solve $\tilde{C}(i\gamma_{\alpha k})$ for all α and k, on top of which we obtain $\tilde{\boldsymbol{X}}_\alpha(\omega)$ from Eq. (43b) and henceforth $\tilde{\boldsymbol{C}}(\omega)$ can be directly gotten from Eq. (43a).

V. SUMMARY

To conclude, we develop the algebraic method to study multimode Brownian oscillators. The algebraic approach directly gives the exact time–local EOM for reduced density operator. Based on this approach, we can easily extract both the reduced system and hybrid bath dynamical informations. We exploit the EOM to study the heat transport and the thermodynamics of quantum mixing, two representative entangled system–bath quantities. It is anticipated that the method developed in this work would constitute a crucial component for nonequilibrium statistical mechanics for open quantum systems, e.g., the network of oscillators. And the DIF method we proposed furnish a basic step to systematically solve the correlation functions of anharmonic system.

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Supplementary materials on "Multimode Brownian oscillators: Thermodynamics and heat transport"

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These supplementary materials on "Multimode Brownian oscillators: Thermodynamics and heat transport" contain (*i*) Detailed derivations of EOM for multimode BO system in Sec. II of the main text; (*ii*) Detailed derivations of cofficients of EOM for HDO; (*iii*) Asymptotic analysis; (*iv*) Theory of heat current, including analysis of equilibrium state and nonequilibrium steady state; (*v*) Detailed derivations of our DIF method.

I. DETAILED DERIVATIONS OF EOM FOR MULTIMODE BO SYSTEM

A. EOM for coordinates and momentums

In this subsection, we derive the time–local equation of motion, Eq. (8) of the main text, followed by EOM of first and second order moments. Let us start from Eq. (5) of the main text, the time–nonlocal EOM. Take the time derivative and we obtain

$$\begin{bmatrix}\dot{\hat{\boldsymbol{Q}}}(t)\\ \dot{\hat{\boldsymbol{P}}}(t)\end{bmatrix} = \dot{\mathbf{T}}(t)\begin{bmatrix}\hat{\boldsymbol{Q}}(0)\\ \hat{\boldsymbol{P}}(0)\end{bmatrix} + \sum_{\alpha}\begin{bmatrix}0\\ \hat{\boldsymbol{F}}^{\rm B}_{\alpha}(t)\end{bmatrix} + \sum_{\alpha}\int_0^t \mathrm{d}\tau\, \dot{\mathbf{T}}(t-\tau)\begin{bmatrix}0\\ \hat{\boldsymbol{F}}^{\rm B}_{\alpha}(\tau)\end{bmatrix}, \tag{S1}$$

by noting that $\mathbf{T}(0)=\mathbf{I}$, the indetity matrix. Equation (5) also implies

$$\begin{bmatrix}\hat{\boldsymbol{Q}}(0)\\ \hat{\boldsymbol{P}}(0)\end{bmatrix} = \mathbf{T}^{-1}(t)\begin{bmatrix}\hat{\boldsymbol{Q}}(t)\\ \hat{\boldsymbol{P}}(t)\end{bmatrix} - \mathbf{T}^{-1}(t)\sum_{\alpha}\int_0^t \mathrm{d}\tau\, \mathbf{T}(t-\tau)\begin{bmatrix}0\\ \hat{\boldsymbol{F}}^{\rm B}_{\alpha}(\tau)\end{bmatrix}. \tag{S2}$$

Substituting Eq. (S2) into the first term on the r.h.s. of Eq. (S1), we obtain

$$\begin{bmatrix}\dot{\hat{\boldsymbol{Q}}}(t)\\ \dot{\hat{\boldsymbol{P}}}(t)\end{bmatrix} = \boldsymbol{\Lambda}(t)\begin{bmatrix}\hat{\boldsymbol{Q}}(t)\\ \hat{\boldsymbol{P}}(t)\end{bmatrix} + \sum_{\alpha}\begin{bmatrix}0\\ \hat{\boldsymbol{F}}^{\rm eff}_{\alpha}(t)\end{bmatrix}. \tag{S3}$$

Here, we define

$$\boldsymbol{\Lambda}(t) \equiv \dot{\mathbf{T}}(t)\mathbf{T}^{-1}(t) \tag{S4}$$

and

$$\begin{bmatrix}0\\ \hat{\boldsymbol{F}}^{\rm eff}_{\alpha}(t)\end{bmatrix} = \begin{bmatrix}0\\ \hat{\boldsymbol{F}}^{\rm B}_{\alpha}(t)\end{bmatrix} + \int_0^t \mathrm{d}\tau\, \boldsymbol{\theta}(t-\tau,t)\begin{bmatrix}0\\ \hat{\boldsymbol{F}}^{\rm B}_{\alpha}(\tau)\end{bmatrix} \tag{S5}$$

with $\boldsymbol{\theta}(\tau,t) \equiv \dot{\mathbf{T}}(\tau) - \boldsymbol{\Lambda}(t)\mathbf{T}(\tau)$. We then obtain the time–local EOM, Eq. (8) of the main text. Equations (9)–(13) are further elaborations of the involved coeffcients.

B. EOM of first and second order moments

In this subsection, the EOM of first and second order moments are derived from Eq. (8). For later use, we denote

$$Q_u(t) \equiv \langle \hat{Q}_u(t)\rangle, \qquad P_u(t) \equiv \langle \hat{P}_u(t)\rangle, \tag{S6}$$

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and

$$W_{uv}^{QQ} \equiv \frac{1}{2}\big\langle\{\delta\hat{Q}_u(t), \delta\hat{Q}_v(t)\}\big\rangle, \quad W_{uv}^{PP} \equiv \frac{1}{2}\big\langle\{\delta\hat{P}_u(t), \delta\hat{P}_v(t)\}\big\rangle, \quad W_{uv}^{QP} \equiv \frac{1}{2}\big\langle\{\delta\hat{Q}_u(t), \delta\hat{P}_v(t)\}\big\rangle, \tag{S7}$$

where $\delta\hat{Q}_u(t) \equiv \hat{Q}_u(t) - Q_u(t)$, $\delta\hat{P}_u(t) \equiv \hat{P}_u(t) - P_u(t)$, and the average, $\langle\cdots\rangle$, is taken over the initial state in the Heisenberg picture. In Eq. (S7), the second order central moments are symmetrized.

Equation (8) with Eqs. (9) and (10) directly gives

$$\dot{Q}_u(t) = P_u(t), \tag{S8a}$$

$$\dot{P}_u(t) = -\sum_v \big[\Omega_{uv}(t)Q_v(t) + \Gamma_{uv}(t)P_v(t)\big] + \sum_\alpha \big\langle \hat{F}^{\rm eff}_{\alpha u}(t)\big\rangle. \tag{S8b}$$

We further adopt the so–called initial factorization ansatz:

$$\rho_{\rm T}(t_0) = \rho_{\rm S}(t_0) \otimes \prod_\alpha \rho_\alpha^{\rm Bbare}(\beta), \quad t_0 = 0, \tag{S9}$$

so that $\big\langle F^{\rm B}_{\alpha u}(t)\big\rangle = {\rm tr}[F^{\rm B}_{\alpha u}(t)\rho_{\rm T}(0)] = \langle F^{\rm B}_{\alpha u}(t)\rangle_{\rm B} = 0$, hence from Eq. (S5) we know In Eq. (S8b) $\big\langle \hat{F}^{\rm eff}_{\alpha u}(t)\big\rangle = 0$ then we get

$$\dot{Q}_u(t) = P_u(t), \tag{S10a}$$

$$\dot{P}_u(t) = -\sum_v \big[\Omega_{uv}(t)Q_v(t) + \Gamma_{uv}(t)P_v(t)\big]. \tag{S10b}$$

Now we turn to second order moments

$$\begin{aligned}\dot{W}_{uv}^{QQ}(t) &= \frac{d}{dt}\langle\frac{\hat{Q}_u(t)\hat{Q}_v(t) + \hat{Q}_v(t)\hat{Q}_u(t)}{2}\rangle - \frac{d}{dt}\big[Q_u(t)Q_v(t)\big] = \frac{1}{2}\langle\hat{P}_u(t)\hat{Q}_v(t)\rangle + \frac{1}{2}\langle\hat{Q}_u(t)\hat{P}_v(t)\rangle - P_u(t)Q_v(t) + (u\leftrightarrow v)\\ &= W_{uv}^{QP}(t) + (u\leftrightarrow v),\end{aligned} \tag{S11}$$

in the second equailty we used Eq. (S10) and in the third equailty we used definitions of second order moments Eq. (S7). By the same method we can also obtain EOM for other second order moments. Then we calculate

$$\dot{W}_{uv}^{PP}(t) = \frac{d}{dt}\langle\frac{P_u(t)P_v(t) + P_v(t)P_u(t)}{2}\rangle - \frac{d}{dt}\big[P_u(t)P_v(t)\big], \tag{S12}$$

first term reads

$$\begin{aligned}&\frac{d}{dt}\langle\frac{P_u(t)P_v(t) + P_v(t)P_u(t)}{2}\rangle\\ &= -\frac{1}{2}\Big\{\sum_{u'}\big[\Omega_{uu'}(t)\langle Q_{u'}(t)P_v(t)\rangle + \Gamma_{uu'}(t)\langle P_{u'}(t)P_v(t)\rangle + \Omega_{vu'}(t)\langle P_u(t)Q_{u'}(t)\rangle + \Gamma_{vu'}(t)\langle P_u(t)P_{u'}(t)\rangle\big]\\ &\qquad - \sum_\alpha\big[\langle F^{\rm eff}_{\alpha u}(t)P_v(t)\rangle + \langle P_u(t)F^{\rm eff}_{\alpha v}(t)\rangle\big]\Big\} + (u\leftrightarrow v),\end{aligned} \tag{S13}$$

second term reads

$$\frac{d}{dt}\big[P_u(t)P_v(t)\big] = -\sum_{u'}\big[\Omega_{uu'}(t)Q_{u'}(t)P_v(t) + \Gamma_{uu'}(t)P_{u'}(t)P_v(t)\big] + (u\leftrightarrow v). \tag{S14}$$

Putting Eq. (S13) and Eq. (S14) into Eq. (S12) we obtain the final result

$$\frac{d}{dt}W_{uv}^{PP}(t) = -\sum_{u'}[\Omega_{uu'}(t)W_{u'v}^{QP}(t) + \Gamma_{uu'}(t)W_{u'v}^{PP}(t)] + \sum_\alpha {\rm Re}\langle F^{\rm eff}_{\alpha u}(t)P_v(t)\rangle + (u\leftrightarrow v). \tag{S15}$$

Finally we turn to $W_{uv}^{QP}(t) \equiv W_{vu}^{PQ}(t)$,

$$\dot{W}_{uv}^{QP}(t) = \frac{d}{dt}\frac{1}{2}\langle\hat{Q}_u(t)\hat{P}_v(t) + \hat{P}_v(t)\hat{Q}_u(t)\rangle - \frac{d}{dt}\langle\hat{Q}_u(t)\rangle\langle\hat{P}_v(t)\rangle, \tag{S16}$$

with

$$\frac{d}{dt}\frac{\langle \hat{Q}_u(t)\hat{P}_v(t)+\hat{P}_v(t)\hat{Q}_u(t)\rangle}{2} = \frac{1}{2}\langle\{\hat{P}_u(t),\hat{P}_v(t)\}\rangle + \sum_\alpha \frac{1}{2}\langle\{\hat{Q}_u(t),\hat{F}^{\rm eff}_{\alpha v}(t)\}\rangle - \frac{1}{2}\sum_{u'}\big[\Omega_{vu'}(t)\langle\{\hat{Q}_u(t),\hat{Q}_{u'}(t)\}\rangle + \Gamma_{vu'}(t)\langle\{\hat{Q}_u(t),\hat{P}_{u'}(t)\}\rangle\big], \tag{S17}$$

and

$$\frac{d}{dt}\big[\hat{Q}_u(t)\hat{P}_v(t)\big] = \hat{P}_u(t)\hat{P}_v(t) - \hat{Q}_u(t)\sum_{u'}\big[\Omega_{vu'}(t)\hat{Q}_{u'}(t)+\Gamma_{vu'}(t)\hat{P}_{u'}(t)\big]. \tag{S18}$$

Putting Eq. (S17) and Eq. (S18) into Eq. (S16) to get the result

$$\dot{W}^{QP}_{uv}(t) = W^{PP}_{uv}(t) - \sum_{u'}\big[\Omega_{vu'}(t)W^{QQ}_{uu'}(t)+\Gamma_{vu'}(t)W^{PQ}_{u'u}(t)\big] + \sum_\alpha {\rm Re}\langle F^{\rm eff}_{\alpha v}(t)Q_u(t)\rangle \tag{S19}$$

also

$$\dot{W}^{PQ}_{uv}(t) = W^{PP}_{vu}(t) - \sum_{u'}\big[\Omega_{uu'}(t)W^{QQ}_{vu'}(t)+\Gamma_{uu'}(t)W^{QP}_{vu'}(t)\big] + \sum_\alpha {\rm Re}\langle F^{\rm eff}_{\alpha u}(t)Q_v(t)\rangle \tag{S20}$$

C. Detailed derivation of Re$\langle\hat{F}^{\rm eff}_{\alpha u}(t)P_v(t)\rangle$ and Re$\langle\hat{F}^{\rm eff}_{\alpha u}(t)Q_v(t)\rangle$

Our aim is to recast Re$\langle\hat{F}^{\rm eff}_{\alpha u}(t)P_v(t)\rangle$ and Re$\langle\hat{F}^{\rm eff}_{\alpha u}(t)Q_v(t)\rangle$ only using response and correlation function of system, bath and system–bath. Firstly we note that the definition of $\hat{\boldsymbol{F}}^{\rm eff}_\alpha(t)$ from Eq. (S4),Eq. (S5) and Eq. (6) from the main text that

$$\begin{aligned}\hat{\boldsymbol{F}}^{\rm eff}_\alpha(t) &= \hat{\boldsymbol{F}}^{\rm B}_\alpha(t) + \int_0^t {\rm d}\tau\,\big[\boldsymbol{\Omega}(t)\boldsymbol{\chi}_{QQ}(t-\tau)+\boldsymbol{\Gamma}(t)\boldsymbol{\chi}_{PQ}(t-\tau)+\dot{\boldsymbol{\chi}}_{PQ}(t-\tau)\big]\hat{\boldsymbol{F}}^{\rm B}_\alpha(\tau)\\ &= \hat{\boldsymbol{F}}^{\rm B}_\alpha(t) + \int_0^t {\rm d}\tau\,\big[\boldsymbol{\Omega}(t)\boldsymbol{\chi}(t-\tau)+\boldsymbol{\Gamma}(t)\dot{\boldsymbol{\chi}}(t-\tau)+\ddot{\boldsymbol{\chi}}(t-\tau)\big]\hat{\boldsymbol{F}}^{\rm B}_\alpha(\tau)\\ &= \hat{\boldsymbol{F}}^{\rm B}_\alpha(t) + \int_0^t {\rm d}\tau\,\boldsymbol{\pi}(t-\tau,t)\hat{\boldsymbol{F}}^{\rm B}_\alpha(\tau),\end{aligned} \tag{S21}$$

where we have denoted $\boldsymbol{\chi}(t)\equiv\{\chi_{uv}(t)=i\langle[Q_u(t),Q_v(0)]\rangle\}$ and

$$\boldsymbol{\pi}(t-\tau,t)\equiv\boldsymbol{\Omega}(t)\boldsymbol{\chi}(t-\tau)+\boldsymbol{\Gamma}(t)\dot{\boldsymbol{\chi}}(t-\tau)+\ddot{\boldsymbol{\chi}}(t-\tau). \tag{S22}$$

By using time–nonlocal equation Eq. (5) in the main text we obtain

$$\begin{aligned}{\rm Re}\langle\hat{F}^{\rm eff}_{\alpha u}(t)\hat{Q}_v(t)\rangle &= \sum_{u_1}{\rm Re}\int_0^t {\rm d}\tau\,\chi_{vu_1}(t-\tau)\langle\hat{F}^{\rm eff}_{\alpha u}(t)\sum_\beta\hat{F}^{\rm B}_{\beta u_1}(\tau)\rangle\\ &= \sum_{u_1}{\rm Re}\int_0^t {\rm d}\tau\,\chi_{vu_1}(t-\tau)\langle\hat{F}^{\rm eff}_{\alpha u}(t)\hat{F}^{\rm B}_{\alpha u_1}(\tau)\rangle.\end{aligned} \tag{S23}$$

Here we used $\big\langle\hat{F}^{\rm eff}_{\alpha u}(t)\hat{Q}_v(0)\big\rangle=0$ and $\big\langle\hat{F}^{\rm B}_{\alpha u}(t)\hat{Q}_v(0)\big\rangle=0$ due to initial factorization ansatz. Put Eq. (S22) into Eq. (S23) we obtain

$$\begin{aligned}{\rm Re}\langle\hat{F}^{\rm eff}_{\alpha u}(t)\hat{Q}_v(t)\rangle &= \sum_{u_1}\int_0^t {\rm d}\tau\,\chi_{vu_1}(t-\tau)a_{\alpha uu_1}(t-\tau) + \sum_{u_1v_1}\int_0^t {\rm d}\tau\,\chi_{vu_1}(t-\tau)\int_0^t {\rm d}\tau_1\,\pi_{uv_1}(t-\tau_1,t)a_{\alpha v_1u_1}(\tau_1-\tau)\\ &= \sum_{u_1}\int_0^t {\rm d}\tau\,\chi_{vu_1}(\tau)a_{\alpha uu_1}(\tau) + \sum_{u_1v_1}\int_0^t {\rm d}\tau\int_0^t {\rm d}\tau_1\,\chi_{vu_1}(\tau)\pi_{uv_1}(\tau_1,t)a_{\alpha v_1u_1}(\tau-\tau_1),\end{aligned} \tag{S24}$$

where we denote $a_{\alpha uv}(t)\equiv{\rm Re}\,c_{\alpha uv}(t)$ to simplify our formulas. Put Eq. (S22) into Eq. (S24) we can organize Eq. (S24) as

$${\rm Re}\langle\hat{F}^{\rm eff}_{\alpha u}(t)\hat{Q}_v(t)\rangle = \sum_{u_1}\int_0^t {\rm d}\tau\,\chi_{vu_1}(\tau)a_{\alpha uu_1}(\tau) + \sum_w\big[\delta_{uw}A^Q_{vw}(t)+\Gamma_{uw}(t)B^Q_{vw}(t)+\Omega_{uw}(t)C^Q_{vw}(t)\big] \tag{S25}$$

with

$$A^Q_{vw}(t) = \sum_{u_1 v_1} \int_0^t \mathrm{d}\tau_1 \int_0^t \mathrm{d}\tau_2\, \chi_{vu_1}(\tau_1) a_{\alpha v_1 u_1}(\tau_1 - \tau_2) \ddot{\chi}_{wv_1}(\tau_2) \tag{S26a}$$

$$B^Q_{vw}(t) = \sum_{u_1 v_1} \int_0^t \mathrm{d}\tau_1 \int_0^t \mathrm{d}\tau_2\, \chi_{vu_1}(\tau_1) a_{\alpha v_1 u_1}(\tau_1 - \tau_2) \dot{\chi}_{wv_1}(\tau_2) \tag{S26b}$$

$$C^Q_{vw}(t) = \sum_{u_1 v_1} \int_0^t \mathrm{d}\tau_1 \int_0^t \mathrm{d}\tau_2\, \chi_{vu_1}(\tau_1) a_{\alpha v_1 u_1}(\tau_1 - \tau_2) \chi_{wv_1}(\tau_2). \tag{S26c}$$

Repeat this procedure to $\mathrm{Re}\langle \hat{F}^{\mathrm{eff}}_{\alpha u}(t) \hat{P}_v(t) \rangle$ we obtain

$$\mathrm{Re}\langle \hat{F}^{\mathrm{eff}}_{\alpha u}(t) \hat{P}_v(t) \rangle = \sum_{u_1} \int_0^t \mathrm{d}\tau\, \dot{\chi}_{vu_1}(\tau) a_{\alpha u u_1}(\tau) + \sum_w \left[\delta_{uw} A^P_{vw}(t) + \Gamma_{uw}(t) B^P_{vw}(t) + \Omega_{uw}(t) C^P_{vw}(t) \right] \tag{S27}$$

with

$$A^P_{vw}(t) = \sum_{u_1 v_1} \int_0^t \mathrm{d}\tau_1 \int_0^t \mathrm{d}\tau_2\, \dot{\chi}_{vu_1}(\tau_1) a_{\alpha v_1 u_1}(\tau_1 - \tau_2) \ddot{\chi}_{wv_1}(\tau_2) \tag{S28a}$$

$$B^P_{vw}(t) = \sum_{u_1 v_1} \int_0^t \mathrm{d}\tau_1 \int_0^t \mathrm{d}\tau_2\, \dot{\chi}_{vu_1}(\tau_1) a_{\alpha v_1 u_1}(\tau_1 - \tau_2) \dot{\chi}_{wv_1}(\tau_2) \tag{S28b}$$

$$C^P_{vw}(t) = \sum_{u_1 v_1} \int_0^t \mathrm{d}\tau_1 \int_0^t \mathrm{d}\tau_2\, \dot{\chi}_{vu_1}(\tau_1) a_{\alpha v_1 u_1}(\tau_1 - \tau_2) \chi_{wv_1}(\tau_2). \tag{S28c}$$

Both Eq. (S26) and Eq. (S28) have similar mathematical structures like

$$T^{ij}_{vw}(t) \overset{\mathrm{def}}{=} \sum_{u_1 v_1} \int_0^t \mathrm{d}\tau_1 \int_0^t \mathrm{d}\tau_2\, \mathcal{D}_i \chi_{vu_1}(\tau_1) a_{\alpha v_1 u_1}(\tau_1 - \tau_2) \mathcal{D}_j \chi_{wv_1}(\tau_2), \tag{S29}$$

where $\mathcal{D}_i \to \mathrm{d}^i/\mathrm{d}t^i$ denotes derivative operator. Therefore we only need to deal with Eq. (S29). But before that we introduce a mathematical identity, for any function $f_1(x), f_2(x)$ and $S(x)$ and denote $L(x) \equiv S(-x)$, we have

$$\begin{aligned}
&\int_0^t \mathrm{d}\tau_1 \int_0^t \mathrm{d}\tau_2\, f_1(\tau_1) S(\tau_1 - \tau_2) f_2(\tau_2) \\
&= \int_0^t \mathrm{d}\tau_2 \int_0^{\tau_2} \mathrm{d}\tau_2\, f_1(\tau_1) S(\tau_1 - \tau_2) f_2(\tau_2) + (1 \leftrightarrow 2) \\
&= \int_0^t \mathrm{d}\tau_2\, f(\tau_2) \int_0^{\tau_2} \mathrm{d}\tau_2\, f_1(\tau_1) S(\tau_1 - \tau_2) + (1 \leftrightarrow 2) \\
&= \int_0^t \mathrm{d}\tau_2\, f(\tau_2) \int_0^{\tau_2} \mathrm{d}\tau_2\, f_1(\tau_1) L(\tau_2 - \tau_1) + (1 \leftrightarrow 2) \\
&= \int_0^t \mathrm{d}\tau\, f_2(\tau) \big[L \otimes f_1 \big](\tau) + (1 \leftrightarrow 2) \\
&= \int_0^t \mathrm{d}\tau\, \big[f_1 \otimes L \big](\tau) f_2(\tau) + \int_0^t \mathrm{d}\tau\, f_1(\tau) \big[L \otimes f_2 \big](\tau),
\end{aligned} \tag{S30}$$

$$\int_0^t \mathrm{d}\tau_1 \int_0^t \mathrm{d}\tau_2\, f_1(\tau_1) S(\tau_1 - \tau_2) f_2(\tau_2) = \int_0^t \mathrm{d}\tau\, f_2(\tau) \big[S \otimes f_1 \big](\tau) + \int_0^t \mathrm{d}\tau\, f_1(\tau) \big[S \otimes f_2 \big](\tau), \tag{S31}$$

the $\otimes$ operator stands for convolve:

$$\big[f \otimes g \big](t) \equiv \int_0^t \mathrm{d}\tau\, f(t - \tau) g(\tau) \equiv \int_0^t \mathrm{d}\tau\, f(\tau) g(t - \tau). \tag{S32}$$

We choose $S(t) = a_{\alpha v_1 u_1}(t)$ and thus $L(t) = a_{\alpha v_1 u_1}(-t) = a_{\alpha u_1 v_1}(t)$ in Eq. (S29) and we can recast Eq. (S29) as

$$T^{ij}_{vw}(t) = \sum_{u_1 v_1} \int_0^t \mathrm{d}\tau\, \mathcal{D}_i \chi_{vu_1}(\tau)\big[a_{\alpha u_1 v_1} \otimes \mathcal{D}_j \chi_{wv_1}\big](\tau) + \int_0^t \mathrm{d}\tau\, \mathcal{D}_j \chi_{wv_1}(\tau)\big[a_{\alpha u_1 v_1} \otimes \mathcal{D}_i \chi_{vu_1}\big](\tau), \tag{S33}$$

for $(i,j) = (0,0),(1,0),(0,1),(1,1),(0,2),(1,2)$. For clarity we further denote(note that $a_{\alpha uv}(t)$ is symmetric.)

$$u_{\alpha uv}(t) = \sum_w \big[\chi_{uw} \otimes a_{\alpha wv}\big](t) = \sum_w \big[\chi_{uw} \otimes a_{\alpha vw}\big](t) = \sum_w \int_0^t \mathrm{d}\tau\, \chi_{uw}(t-\tau) a_{\alpha wv}(\tau). \tag{S34}$$

It is obvious that

$$\dot{u}_{\alpha uv}(t) = \sum_w \int_0^t \mathrm{d}\tau\, \dot{\chi}_{uw}(t-\tau) a_{\alpha wv}(\tau) = \sum_w \big[\mathcal{D}_1 \chi_{uw} \otimes a_{\alpha wv}\big](t) \tag{S35}$$

and

$$\ddot{u}_{\alpha uv}(t) = a_{\alpha uv}(t) + \sum_w \int_0^t \mathrm{d}\tau\, \ddot{\chi}_{uw}(t-\tau) a_{\alpha wv}(\tau) = a_{\alpha vu}(t) + \sum_w \big[\mathcal{D}_2 \chi_{uw} \otimes a_{\alpha wv}\big](t), \tag{S36}$$

Eq. (S34), Eq. (S35) and Eq. (S36) can be organized into a compact form

$$\mathcal{D}_i u_{\alpha uv}(t) = \delta_{i,2} a_{\alpha uv}(t) + \sum_w \big[\mathcal{D}_i \chi_{uw} \otimes a_{\alpha vw}\big](t), \tag{S37}$$

substitude it into Eq. (S29) we get for $(i,j) = (0,0),(1,0),(0,1),(1,1),(0,2),(1,2)$

$$\text{if } j \neq 2 \quad T^{ij}_{vw}(t) = \sum_{u_1} \int_0^t \mathrm{d}\tau\, \big[\mathcal{D}_i \chi_{vu_1}(\tau) \mathcal{D}_j u_{\alpha wu_1}(\tau) + \mathcal{D}_j \chi_{wu_1}(\tau) \mathcal{D}_i u_{\alpha vu_1}(\tau)\big] \tag{S38a}$$

$$\text{if } j = 2 \quad T^{ij}_{vw}(t) = \sum_{u_1} \int_0^t \mathrm{d}\tau\, \big[\mathcal{D}_i \chi_{vu_1}(\tau) \mathcal{D}_j u_{\alpha wu_1}(\tau) + \mathcal{D}_j \chi_{wu_1}(\tau) \mathcal{D}_i u_{\alpha vu_1}(\tau)\big] - \sum_{u_1} \int_0^t \mathrm{d}\tau\, \mathcal{D}_i \chi_{vu_1}(\tau) a_{\alpha u_1 w}(\tau), \tag{S38b}$$

note that the last term in Eq. (S38b) will cancel out the first term in both Eq. (S25)(when $i = 0$) and Eq. (S27)(when $i = 1$):

$$\begin{aligned}
&\sum_{u_1} \int_0^t \mathrm{d}\tau\, \mathcal{D}_i \chi_{vu_1}(\tau) a_{\alpha uu_1}(\tau) - \sum_w \delta_{uw} \sum_{u_1} \int_0^t \mathrm{d}\tau\, \mathcal{D}_i \chi_{vu_1}(\tau) a_{\alpha u_1 w}(\tau) \\
&= \sum_{u_1} \int_0^t \mathrm{d}\tau\, \mathcal{D}_i \chi_{vu_1}(\tau) \big[a_{\alpha uu_1}(\tau) - a_{\alpha u_1 u}(\tau)\big] \\
&= 0,
\end{aligned} \tag{S39}$$

since $\tilde{\phi}_\alpha(\omega)$ is symmetrical and from fluctuation-dissipation theorem

$$c^{(+)}_{\alpha uv}(\omega) = \frac{\tilde{\phi}^{(-)}_{\alpha uv}(\omega)}{1 - e^{-\beta_\alpha \omega}}, \tag{S40}$$

where $(-)$ denotes the anti-Hermitian part of the matrix while $(+)$ denotes the Hermitian part. We know $a_{\alpha uv}(t) \equiv \mathrm{Re}\, c^{(+)}_{\alpha uv}(t)$ is also symmetrical. After putting Eq. (S38) into Eq. (S25) and Eq. (S27) we we will find

$$\mathrm{Re}\langle \hat{F}^{\mathrm{eff}}_{\alpha u}(t) \hat{Q}_v(t)\rangle = \sum_w \big[\Omega_{uw} k^{00}_{\alpha vw}(t) + \Gamma_{uw}(t) k^{01}_{\alpha vw}(t) + \delta_{uw} k^{02}_{\alpha vw}(t)\big] \tag{S41a}$$

$$\mathrm{Re}\langle \hat{F}^{\mathrm{eff}}_{\alpha u}(t) \hat{P}_v(t)\rangle = \sum_w \big[\Omega_{uw} k^{10}_{\alpha vw}(t) + \Gamma_{uw}(t) k^{11}_{\alpha vw}(t) + \delta_{uw} k^{12}_{\alpha vw}(t)\big], \tag{S41b}$$

with

$$k^{ij}_{\alpha vw}(t) = \sum_{u_1} \int_0^t \mathrm{d}\tau\, \big[\mathcal{D}_i \chi_{vu_1}(\tau) \mathcal{D}_j u_{\alpha wu_1}(\tau) + \mathcal{D}_j \chi_{wu_1}(\tau) \mathcal{D}_i u_{\alpha vu_1}(\tau)\big], \tag{S42}$$

or in a matrix form

$$\boldsymbol{k}_{\alpha}^{ij}(t)=\int_0^t \mathrm{d}\tau\,\big[\mathcal{D}_i\boldsymbol{\chi}(\tau)\mathcal{D}_j\boldsymbol{u}_{\alpha}^{\mathrm{T}}(\tau)+\mathcal{D}_i\boldsymbol{u}_{\alpha}(\tau)\mathcal{D}_j\boldsymbol{\chi}^{\mathrm{T}}(\tau)\big], \tag{S43}$$

and the final results read(here we introduce Eq. (S57) and Eq. (S61) to simplify notation.)

$$\begin{bmatrix}\boldsymbol{\gamma}_{\alpha}'(t) & \boldsymbol{\gamma}_{\alpha}(t)\end{bmatrix}=\begin{bmatrix}\boldsymbol{\Omega}(t) & \boldsymbol{\Gamma}(t) & \mathbf{I}\end{bmatrix}\begin{bmatrix}\boldsymbol{k}_{\alpha00}^{\mathrm{T}}(t) & \boldsymbol{k}_{\alpha10}^{\mathrm{T}}(t)\\ \boldsymbol{k}_{\alpha01}^{\mathrm{T}}(t) & \boldsymbol{k}_{\alpha11}^{\mathrm{T}}(t)\\ \boldsymbol{k}_{\alpha02}^{\mathrm{T}}(t) & \boldsymbol{k}_{\alpha12}^{\mathrm{T}}(t)\end{bmatrix}, \tag{S44}$$

from Eq. (S43) we know

$$\big[\boldsymbol{k}_{\alpha}^{ij}(t)\big]^{\mathrm{T}}=\boldsymbol{k}_{\alpha}^{ji}(t) \tag{S45}$$

II. COEFFICIENTS OF EOM OF HDO

A. First order moments,derivation of $\Gamma_{\alpha uv}$ and $\Omega_{\alpha uv}$

We rederive the first and second order moments using EOM of HDO, Eq. motionrho, and compare the results with that from time–local EOM to obtain the coefficients. From Eq. (14),Eq. (17a) and Eq. (17b), we can obtain

$$\begin{aligned}\dot{Q}_u(t)=&\mathrm{tr}\big[Q_u\dot{\rho}_{\mathrm{S}}(t)\big]\\ =&\mathrm{tr}\Big(Q_u\Big\{-i\big[\sum_{u'}\frac{\hat{P}_{u'}^2}{2}+\frac{1}{2}\sum_{u'v}V_{uv}\hat{Q}_{u'}\hat{Q}_v,\rho_{\mathrm{S}}(t)\big]-i\sum_{\alpha u'}\big[\hat{Q}_{u'},\varrho_{\alpha u'}(t)\big]\Big\}\Big)\\ =&-i\mathrm{tr}(Q_u\big[\sum_{u'}\frac{\hat{P}_{u'}^2}{2},\rho_{\mathrm{S}}(t)\big])\\ =&P_u(t),\end{aligned} \tag{S46}$$

which agrees with time–local EOM. Note that $\mathrm{tr}(\hat{Q}_u[\hat{Q}_v,\varrho_{\alpha v}(t)])\equiv 0$ for any u and v. Then we calculate

$$\begin{aligned}\dot{P}_u(t)=&\mathrm{tr}\big[\hat{P}_u\dot{\rho}_{\mathrm{S}}(t)\big]\\ =&\mathrm{tr}(\hat{P}_u-i\Big[\sum_{u'}\frac{\hat{P}_{u'}^2}{2}+\frac{1}{2}\sum_{u'v}V_{uv}\hat{Q}_{u'}\hat{Q}_v,\rho_{\mathrm{S}}(t)\Big]-i\sum_{\alpha u'}[\hat{Q}_{u'},\varrho_{\alpha u'}(t)])\\ =&-\sum_v\frac{1}{2}(V_{uv}+V_{vu})Q_v(t)-\sum_{\alpha v}\mathrm{tr}\big[\Omega_{\alpha uv}(t)Q_v^{\oplus}\rho_{\mathrm{S}}(t)\big]-\sum_{\alpha v}\mathrm{tr}\big[\Gamma_{\alpha uv}(t)P_v^{\oplus}\rho_{\mathrm{S}}(t)\big]\\ =&-\sum_v\frac{1}{2}(V_{uv}+V_{vu})Q_v(t)-\sum_{\alpha v}\Omega_{\alpha uv}(t)Q_v(t)-\sum_{\alpha v}\Gamma_{\alpha uv}(t)P_v(t),\end{aligned} \tag{S47}$$

compare it with Eq. (S10b) we know that

$$\sum_{\alpha}\Omega_{\alpha uv}(t)=\Omega_{uv}(t)-\frac{1}{2}(V_{uv}+V_{vu}) \tag{S48a}$$

$$\sum_{\alpha}\Gamma_{\alpha uv}(t)=\Gamma_{uv}(t), \tag{S48b}$$

we can always make $\boldsymbol{V}$ matrix symmetry so that

$$\sum_{\alpha}\Omega_{\alpha uv}(t)=\Omega_{uv}(t)-V_{uv}, \tag{S49a}$$

$$\sum_{\alpha}\Gamma_{\alpha uv}(t)=\Gamma_{uv}(t). \tag{S49b}$$

B. Second order moments,derivation of $\gamma_{\alpha uv}$ and $\gamma'_{\alpha uv}$

Again from Eq. (14), Eq. (17a) and Eq. (17b) we can obtain

$$\begin{aligned}
\dot{W}^{QQ}_{uv}(t) =& \frac{d}{dt}\langle\frac{\hat{Q}_u(t)\hat{Q}_v(t)+\hat{Q}_v(t)\hat{Q}_u(t)}{2}\rangle - \frac{d}{dt}\big[Q_u(t)Q_v(t)\big] \\
=& - i\mathrm{tr}\Big(\frac{\hat{Q}_u\hat{Q}_v+\hat{Q}_v\hat{Q}_u}{2}\big[\frac{1}{2}\big(\sum_{u'}\hat{P}^2_{u'}+\sum_{u'v'}V_{u'v'}\hat{Q}_{u'}\hat{Q}_{v'}\big),\rho_{\mathrm{S}}(t)\big]\Big) - \frac{d}{dt}\big[Q_u(t)Q_v(t)\big] \\
=& \frac{1}{2}\big\langle\hat{Q}_u(t)\hat{P}_v(t)+\hat{P}_u(t)\hat{Q}_v(t)\big\rangle - P_u(t)Q_v(t) + (u\leftrightarrow v) \\
=& \frac{1}{2}\langle\{\delta\hat{P}_u(t),\delta\hat{Q}_v(t)\}\rangle + (u\leftrightarrow v),
\end{aligned} \tag{S50}$$

which also agrees with Eq. (S11). Then we calculate

$$\begin{aligned}
\dot{W}^{PP}_{uv}(t) =& \frac{d}{dt}\langle\frac{\hat{P}_u(t)\hat{P}_v(t)+\hat{P}_v(t)\hat{P}_u(t)}{2}\rangle - \frac{d}{dt}\big[P_u(t)P_v(t)\big] \\
=& - i\mathrm{tr}\Big(\frac{\hat{P}_u\hat{P}_v+\hat{P}_v\hat{P}_u}{2}\big[\frac{1}{2}\big(\sum_{u'}\hat{P}^2_{u'}+\sum_{u'v'}V_{u'v'}\hat{Q}_{u'}\hat{Q}_{v'}\big),\rho_{\mathrm{S}}(t)\big]\Big) - \frac{d}{dt}\big[P_u(t)P_v(t)\big],
\end{aligned} \tag{S51}$$

which contains four terms and all of them needs tedious but trivial calculation, we only briefly show some key steps. First term from H_{S} reads

$$\begin{aligned}
& - i\mathrm{tr}\big(\frac{\hat{P}_u\hat{P}_v+\hat{P}_v\hat{P}_u}{2}\big[\frac{1}{2}\big(\sum_{u'}\hat{P}^2_{u'}+\sum_{u'v'}V_{u'v'}\hat{Q}_{u'}\hat{Q}_{v'}\big),\rho_{\mathrm{S}}(t)\big]\big) \\
=& -\frac{1}{2}\sum_{u'}\big\langle V_{uu'}\hat{P}_v(t)\hat{Q}_{u'}(t)+V_{vu'}\hat{P}_u(t)\hat{Q}_{u'}(t)+V_{u'u}\hat{Q}_{u'}(t)\hat{P}_v(t)+V_{u'v}\hat{Q}_{u'}(t)\hat{P}_u(t)\big\rangle \\
=& -\frac{1}{2}\sum_{u'}\big[V_{uu'}\big\langle\{\hat{P}_v(t),\hat{Q}_{u'}(t)\}\big\rangle+V_{vu'}\big\langle\{\hat{P}_u(t),\hat{Q}_{u'}(t)\}\big\rangle\big] \\
=& -\frac{1}{2}\sum_{u'}V_{uu'}\big\langle\{\hat{P}_v(t),\hat{Q}_{u'}(t)\}\big\rangle + (u\leftrightarrow v),
\end{aligned} \tag{S52}$$

note that$[P_u(t)P_v(t),Q_{u'}(t)Q_{v'}(t)] = -i[P_u(t)\delta_{vu'}+\delta_{uu'}P_v(t)]Q_{v'}(t)+Q_{u'}(t)[P_u(t)\delta_{vv'}+\delta_{uv'}P_v(t)]$. Second term:

$$\begin{aligned}
& - i\mathrm{tr}\Big(\frac{P_uP_v+P_vP_u}{2}\sum_{\alpha u'v'}\big[Q_{u'},\varrho^{(1)}_{\alpha u'v'}(t)\big]\Big) \\
=& \sum_{\alpha u'v'} -i\mathrm{tr}\Big(\frac{P_uP_v+P_vP_u}{2}[Q_{u'},\big(\Omega_{\alpha u'v'}(t)Q^{\oplus}_{v'}+\Gamma_{\alpha u'v'}(t)P^{\oplus}_{v'}\big)\rho_{\mathrm{S}}]\Big) \\
=& -\frac{1}{4}\sum_{\alpha v'}\big\langle\{\Omega_{\alpha vv'}(t)\hat{P}_u(t)+\Omega_{\alpha uv'}(t)\hat{P}_v(t),\hat{Q}_{v'}(t)\}\big\rangle - \frac{1}{4}\sum_{\alpha u'v'}\Gamma_{\alpha u'v'}(t)\big\langle\{\hat{P}_u(t)\delta_{vu'}+\delta_{uu'}\hat{P}_v(t),\hat{P}_{v'}(t)\}\big\rangle + (u\leftrightarrow v) \\
=& -\frac{1}{2}\sum_{\alpha u'}\Omega_{\alpha vu'}(t)\big\langle\{\hat{P}_u(t),\hat{Q}_{u'}(t)\}\big\rangle - \frac{1}{2}\sum_{\alpha u'}\Gamma_{\alpha vu'}(t)\big\langle\{\hat{P}_u(t),\hat{P}_{u'}(t)\}\big\rangle + (u\leftrightarrow v),
\end{aligned} \tag{S53}$$

The third term:

$$\begin{aligned}
-i\mathrm{tr}\Big(\frac{\hat{P}_u\hat{P}_v+\hat{P}_v\hat{P}_u}{2}\sum_{\alpha u'v'}[\hat{Q}_{u'},\varrho^{(2)}_{\alpha u'v'}]\Big) =& -\frac{1}{2}\mathrm{tr}\sum_{\alpha u'v'}\big[(\hat{P}_u\delta_{vu'}+\delta_{uu'}\hat{P}_v)(\gamma_{\alpha u'v'}(t)\hat{Q}^{\ominus}_{v'})\rho_{\mathrm{S}}(t)\big] + (u\leftrightarrow v) \\
=& \sum_{\alpha}\gamma_{\alpha uv}(t) + (u\leftrightarrow v),
\end{aligned} \tag{S54}$$

Sum them up, we get the final result for $\frac{d}{dt}\langle\frac{\hat{P}_u(t)\hat{P}_v(t)+\hat{P}_v(t)\hat{P}_u(t)}{2}\rangle$

$$\begin{aligned}
\frac{d}{dt}\langle\frac{\hat{P}_u(t)\hat{P}_v(t)+\hat{P}_v(t)\hat{P}_u(t)}{2}\rangle =& -\frac{1}{2}\sum_{u'}\Omega_{vu'}(t)\langle\{\hat{P}_u(t),\hat{Q}_{u'}(t)\}\rangle - \frac{1}{2}\sum_{u'}\Gamma_{vu'}(t)\langle\{\hat{P}_u(t),\hat{P}_{u'}(t)\}\rangle + \sum_{\alpha}\gamma_{\alpha uv}(t) \\
& + (u\leftrightarrow v)
\end{aligned} \tag{S55}$$

we have used Eq. (S49a) here, subsribe it into Eq. (S51) and using Eq. (S47) we can obtain

$$\dot{W}^{PP}_{uv}(t) = -\sum_{u'}\left[\Omega_{uu'}(t)W^{QP}_{u'v}(t) + \Gamma_{uu'}(t)W^{PP}_{u'v}(t)\right] + \sum_{\alpha}\gamma_{\alpha uv}(t) + (u \leftrightarrow v). \tag{S56}$$

If we compare the expression Eq. (S56) with Eq. (S15) we will identify that

$$\gamma_{\alpha uv}(t) = \mathrm{Re}\big\langle F^{\mathrm{eff}}_{\alpha u}(t)P_v(t)\big\rangle. \tag{S57}$$

Similarly we deal with $W^{QP}_{uv}(t)$,

$$\begin{aligned}\dot{W}^{QP}_{uv}(t) &= \frac{d}{dt}\langle\frac{\hat{Q}_u(t)\hat{P}_v(t) + \hat{P}_v(t)\hat{Q}_u(t)}{2}\rangle - \frac{d}{dt}\big[Q_u(t)P_v(t)\big],\\ &= -i\mathrm{tr}\Big(\frac{\hat{Q}_u\hat{P}_v + \hat{P}_v\hat{Q}_u}{2}\big[\frac{1}{2}\big(\sum_{u'}\hat{P}^2_{u'} + \sum_{u'v'}V_{u'v'}\hat{Q}_{u'}\hat{Q}_{v'}\big), \rho_{\mathrm{S}}(t)\big]\Big) - \frac{d}{dt}\big[Q_u(t)P_v(t)\big]\end{aligned} \tag{S58}$$

where

$$\begin{aligned}&\frac{d}{dt}\langle\frac{\hat{P}_u(t)\hat{Q}_v(t) + \hat{Q}_v(t)\hat{P}_u(t)}{2}\rangle\\ =&-i\mathrm{tr}\Big(\frac{\hat{P}_u\hat{Q}_v + \hat{Q}_v\hat{P}_u}{2}\big[\frac{1}{2}\big(\sum_{u'}\hat{P}^2_{u'} + \sum_{u'v'}V_{u'v'}\hat{Q}_{u'}\hat{Q}_{v'}\big), \rho_{\mathrm{S}}(t)\big]\Big)\\ =&\frac{1}{2}\big\langle\{\hat{P}_u(t), \hat{P}_v(t)\}\big\rangle - \frac{1}{2}\sum_{u'}(V_{vu'} + V_{u'v})\big\langle\hat{Q}_u(t)\hat{Q}_{u'}(t)\big\rangle - \frac{1}{2}\sum_{\alpha u'}\Omega_{\alpha vu'}\mathrm{tr}(\hat{Q}_u\{\hat{Q}_{u'}, \rho_{\mathrm{S}}(t)\})\\ &-\frac{1}{2}\sum_{\alpha u'v'}\Gamma_{\alpha u'v'}(t)\mathrm{tr}(\hat{Q}_u\delta_{vu'}\{\hat{P}_{v'}, \rho_{\mathrm{S}}(t)\}) + \frac{1}{2}\sum_{\alpha u'v'}\gamma'_{\alpha u'v'}(t)\mathrm{tr}\Big((-i\delta_{vu'}\hat{Q}_u - i\delta_{vu'}\hat{Q}_u)\big[\hat{P}_{v'}, \rho_{\mathrm{S}}(t)\big]\Big)\\ =&\frac{1}{2}\big\langle\{\hat{P}_u(t), \hat{P}_v(t)\}\big\rangle - \frac{1}{2}\sum_{u'}\Omega_{vu'}(t)\big\langle\hat{Q}_u(t)\hat{Q}_{u'}(t)\rangle + \sum_{\alpha}\gamma'_{\alpha vu}(t) - \frac{1}{2}\sum_{u'}\Gamma_{vu'}(t)\langle\{\hat{Q}_u(t), \hat{P}_{u'}(t)\}\rangle,\end{aligned} \tag{S59}$$

and use basic calculation to get

$$\dot{W}^{QP}_{uv}(t) = W^{PP}_{uv}(t) - \sum_{u'}\Omega_{vu'}(t)W^{QQ}_{uu'}(t) + \sum_{\alpha}\gamma'_{\alpha vu}(t) - \sum_{u'}\Gamma_{vu'}(t)W^{PQ}_{u'u}(t) \tag{S60}$$

we can exam it term by term and compare it with the result of time-local EOM, Eq. (S16) to find they are equal and indentify that

$$\gamma'_{\alpha uv}(t) = \mathrm{Re}\big\langle F^{\mathrm{eff}}_{\alpha u}(t)Q_v(t)\big\rangle, \tag{S61}$$

C. exciplit expressions for $\Omega_{\alpha uv}(t)$ and $\Gamma_{\alpha uv}(t)$

In this part we will give a detailed equation for $\mathbf{\Gamma}(t)$ and $\mathbf{\Omega}(t)$ attributed to each baths, which will be very useful for numerical verification and buliding connection with nonequilibrium thermodynamics.

From Eq. (8) with Eq. (9) and Eq. (10) we can reformulate $\dot{\mathbf{T}}(t)$ matirx as

$$\dot{\chi}^{QP}_{uv}(t) = \chi^{PP}_{uv}(t) \tag{S62a}$$

$$\dot{\chi}^{QQ}_{uv}(t) = \chi^{PQ}_{uv}(t) \tag{S62b}$$

$$\dot{\chi}^{PP}_{uv}(t) = -\sum_{k}V_{uk}\chi^{QP}_{kv}(t) + i\sum_{\alpha}\langle[\hat{F}_{\alpha u}(t), \hat{P}_v(0)]\rangle \tag{S62c}$$

$$\dot{\chi}^{PQ}_{uv}(t) = -\sum_{k}V_{uk}\chi^{QQ}_{kv}(t) + i\sum_{\alpha}\langle[\hat{F}_{\alpha u}(t), \hat{Q}_v(0)]\rangle, \tag{S62d}$$

from Eq. (2) we easily get

$$\dot{\chi}^{PP}_{uv}(t) = -\sum_{k}V_{uk}\chi^{QP}_{kv}(t) + \sum_{\alpha k}\int_0^t \mathrm{d}\tau\,\phi_{\alpha uk}(t-\tau)\chi^{QP}_{kv}(\tau) \tag{S63a}$$

$$\dot{\chi}^{PQ}_{uv}(t) = -\sum_{k}V_{uk}\chi^{QQ}_{kv}(t) + \sum_{\alpha k}\int_0^t \mathrm{d}\tau\,\phi_{\alpha uk}(t-\tau)\chi^{QQ}_{kv}(\tau) \tag{S63b}$$

Thus we have

$$\dot{\mathbf{T}}(t) = \begin{bmatrix} 0 & \boldsymbol{I} \\ -\boldsymbol{V} & 0 \end{bmatrix} \begin{bmatrix} -\boldsymbol{\chi}_{QP}(t) & \boldsymbol{\chi}_{QQ}(t) \\ -\boldsymbol{\chi}_{PP}(t) & \boldsymbol{\chi}_{PQ}(t) \end{bmatrix} + \sum_{\alpha} \int_0^t \mathrm{d}\tau \begin{bmatrix} 0 & 0 \\ \tilde{\boldsymbol{\phi}}_{\alpha}(t-\tau) & 0 \end{bmatrix} \begin{bmatrix} -\boldsymbol{\chi}_{QP}(t) & \boldsymbol{\chi}_{QQ}(t) \\ -\boldsymbol{\chi}_{PP}(t) & \boldsymbol{\chi}_{PQ}(t) \end{bmatrix} \tag{S64}$$

this means

$$\dot{\mathbf{T}}(t) = \begin{bmatrix} 0 & \boldsymbol{I} \\ -\boldsymbol{V} & 0 \end{bmatrix} \mathbf{T}(t) + \sum_{\alpha} \int_0^t \mathrm{d}\tau \begin{bmatrix} 0 & 0 \\ \tilde{\boldsymbol{\phi}}_{\alpha}(t-\tau) & 0 \end{bmatrix} \mathbf{T}(\tau), \tag{S65}$$

using Eq. (9) we can recast $\boldsymbol{\Lambda}(t)$ matrix as

$$\boldsymbol{\Lambda}(t) = \begin{bmatrix} 0 & \boldsymbol{I} \\ -\boldsymbol{V} & 0 \end{bmatrix} + \sum_{\alpha} \int_0^t \mathrm{d}\tau \begin{bmatrix} 0 & 0 \\ \tilde{\boldsymbol{\phi}}_{\alpha}(t-\tau) & 0 \end{bmatrix} \mathbf{T}(\tau)\mathbf{T}^{-1}(t) \tag{S66}$$

which from Eq. (10a)–Eq. (10d) and Eq. (S49) gives us

$$\begin{bmatrix} \boldsymbol{\Omega}_{\alpha}(t) \\ \boldsymbol{\Gamma}_{\alpha}(t) \end{bmatrix}^T = -\int_0^t \mathrm{d}\tau \begin{bmatrix} \tilde{\boldsymbol{\phi}}_{\alpha}(t-\tau) \\ 0 \end{bmatrix}^T \mathbf{T}(\tau)\mathbf{T}^{-1}(t), \tag{S67}$$

III. ASYMPTOTIC ANALYSIS

Here are our building blocks of this section, namely we will convert any response function to $\boldsymbol{\chi}$

$$\boldsymbol{\chi}^{PQ}(t) \equiv \dot{\boldsymbol{\chi}}(t) \tag{S68a}$$
$$\dot{\boldsymbol{\chi}}^{PQ}(t) \equiv \ddot{\boldsymbol{\chi}}(t) \tag{S68b}$$
$$\boldsymbol{\chi}^{PP}(t) \equiv -\ddot{\boldsymbol{\chi}}(t) \tag{S68c}$$
$$\dot{\boldsymbol{\chi}}^{PP}(t) \equiv -\dddot{\boldsymbol{\chi}}(t) \tag{S68d}$$
$$\boldsymbol{\chi}^{QP}(t) \equiv -\dot{\boldsymbol{\chi}}(t) \tag{S68e}$$

A. asymptotic behaviour of response function

Then we can move forward to get many useful result:

$$\boldsymbol{\chi}(0) = \mathbf{0}, \tag{S69}$$

This is trivial

$$\dot{\boldsymbol{\chi}}(0) = \boldsymbol{I}, \tag{S70}$$

This is because $\chi_{uv}(0) = i\langle[\dot{\hat{Q}}_u(0), \hat{Q}_v(0)]\rangle = i\langle[\hat{P}_u(0), \hat{Q}_v(0)]\rangle = \delta_{uv}$

$$\boldsymbol{\chi}^{\mathrm{SB}}_{\alpha}(0) = \boldsymbol{\chi}^{\mathrm{BS}}_{\alpha}(0) = \mathbf{0} \tag{S71}$$

Note that at $t = 0$, $\hat{F}_{\alpha v}(0)$ they commutes with system operators.

$$\ddot{\boldsymbol{\chi}}(0) = \mathbf{0}, \tag{S72}$$

We use $\ddot{\boldsymbol{\chi}}(0) = -\boldsymbol{\Omega}\boldsymbol{V}\boldsymbol{\chi}(0) + \boldsymbol{\Omega}\boldsymbol{\chi}^{\mathrm{BS}}(0) = \mathbf{0}$

$$\boldsymbol{\chi}^{\mathrm{BB}} = \mathbf{0}, \tag{S73}$$

Also trivial

$$\dot{\boldsymbol{\chi}}^{\mathrm{SB}}_{\alpha}(0) = \mathbf{0}, \tag{S74}$$

We know $\dot{\boldsymbol{\chi}}^{\text{SB}}_{\alpha uv}(0) = i\langle[\dot{Q}_u(0), \dot{F}_{\alpha v}(0)]\rangle = \mathbf{0}$

$$\dddot{\chi}^{\text{SB}}_{\alpha}(0) = \mathbf{0}, \tag{S75}$$

We use $\ddot{\boldsymbol{\chi}}^{\text{SB}}_{\alpha}(0) = -\boldsymbol{V}\boldsymbol{\chi}^{\text{SB}}_{\alpha}(0) + \boldsymbol{\chi}^{\text{BB}}_{\alpha}(0) = \mathbf{0}$ Then we turn to calculate $\dddot{\boldsymbol{\chi}}(0), \ddddot{\boldsymbol{\chi}}(0), d^5\boldsymbol{\chi}/d^5t\Big|_{t=0}$ First we have

$$\dddot{\hat{Q}}_u(t) = -\sum_v V_{uv}\dot{\hat{Q}}_v(t) + \sum_\alpha \dot{\hat{F}}^{\text{B}}_{\alpha u}(t)\sum_{\alpha v}\phi_{\alpha uv}(0)\hat{Q}_v(t) + \sum_{\alpha v}\int_0^t \mathrm{d}\tau\, \dot{\phi}_{\alpha uv}(t-\tau)\hat{Q}_v(\tau), \tag{S76}$$

Note that $\phi_{\alpha uv}(0) = 0$ from Eq. (3), the last term vanishes and the second term wil not contribute in following calculation

$$\dddot{\chi}_{uv}(0) = i\langle[-\sum_{v_1} V_{uu'}\hat{P}_{u'}(0), \hat{Q}_v(0)]\rangle = -V_{uv}, \tag{S77}$$

so that

$$\dddot{\boldsymbol{\chi}}(0) = -\boldsymbol{V}, \tag{S78}$$

then we know

$$\ddddot{\hat{Q}}_u(0) = -(\sum_v V_{uv}\ddot{\hat{Q}}_v(0) + \sum_{\alpha v}\dot{\phi}_{\alpha uv}(0)\hat{Q}_v(0)) \tag{S79}$$

note that $\ddot{\hat{Q}}_v(0) = -\sum_{u'} V_{vu'}\hat{Q}_{u'}(0) + \sum_\alpha \hat{F}^{\text{B}}_{\alpha v}(0)$ so it will not commute We get

$$\ddddot{\boldsymbol{\chi}}(0) = \mathbf{0}. \tag{S80}$$

The $d^5\boldsymbol{\chi}/d^5t\Big|_{t=0}$ is much more complex, First take derivative of Eq. (S79) we can calculate

$$\begin{aligned}
\frac{d^5}{dt^5}\chi_{uv}\Big|_{t=0} &= \big\langle -\sum_{u'} V_{uu'}\dddot{\hat{Q}}_{u'}(0) + \sum_{\alpha u'}\dot{\phi}_{\alpha uu'}(0)\dot{\hat{Q}}_{u'}(0) + \sum_{\alpha u'}\ddot{\phi}_{\alpha uu'}(0)\hat{Q}_{u'}(t), \hat{Q}_v(0)\big\rangle \\
&= \sum_{v_1 v_2} V_{uv_1}V_{v_1v_2}\dot{\chi}_{v_2v}(0) + \sum_{\alpha v}\dot{\phi}_{\alpha uv_1}(0)\dot{\chi}_{v_1v}(0) \\
&= \sum_{v_1} V_{uv_1}V_{v_1v} + \sum_\alpha \dot{\phi}_{\alpha uv}(0),
\end{aligned} \tag{S81}$$

so that

$$d^5\boldsymbol{\chi}/d^5t\Big|_{t=0} = \boldsymbol{V}^2 + \sum_\alpha \dot{\boldsymbol{\phi}}(0) \tag{S82}$$

then we come to the quantity $\boldsymbol{\chi}^{\text{BB}}_{\alpha}(0)$ We get

$$\ddot{\hat{F}}_{\alpha u}(0) = \ddot{\hat{F}}^{\text{B}}_{\alpha u}(0) + \sum_{u'}\phi_{\alpha uu'}\hat{Q}_{u'}(0), \tag{S83}$$

so that $\ddot{\boldsymbol{\chi}}^{\text{BB}}_{\alpha}(0) = \ddot{\boldsymbol{\phi}}_\alpha(0) = 0$,obviously $\dot{\boldsymbol{\chi}}^{\text{BB}}_{\alpha}(0) = \dot{\boldsymbol{\phi}}_\alpha(0)$.

B. asymptotic behaviour of Ω_{uv} and Γ_{uv}

In this subsection we omit t argument when necessary for clarity, from Eq. (10a)–Eq. (10d) and Eq. (13) we get

$$\begin{aligned}
\boldsymbol{\Omega}(t) &= -\dddot{\boldsymbol{\chi}}\big[\boldsymbol{\chi}(\dot{\boldsymbol{\chi}})^{-1}(-\ddot{\boldsymbol{\chi}}) + \dot{\boldsymbol{\chi}}\big]^{-1} - \ddot{\boldsymbol{\chi}}\big[\boldsymbol{\chi} + \dot{\boldsymbol{\chi}}(-\ddot{\boldsymbol{\chi}})^{-1}\dot{\boldsymbol{\chi}}\big]^{-1} \\
&= \big[\dddot{\boldsymbol{\chi}}(\boldsymbol{\chi}\dot{\boldsymbol{\chi}}^{-1}\ddot{\boldsymbol{\chi}} - \dot{\boldsymbol{\chi}})^{-1} - \ddot{\boldsymbol{\chi}}(\boldsymbol{\chi} - \dot{\boldsymbol{\chi}}\ddot{\boldsymbol{\chi}}^{-1}\dot{\boldsymbol{\chi}})^{-1}\big],
\end{aligned} \tag{S84}$$

similarly

$$\boldsymbol{\Gamma}(t) = \dddot{\boldsymbol{\chi}}(\dot{\boldsymbol{\chi}}\boldsymbol{\chi}^{-1}\dot{\boldsymbol{\chi}} - \ddot{\boldsymbol{\chi}})^{-1} - \ddot{\boldsymbol{\chi}}(\dot{\boldsymbol{\chi}} - \ddot{\boldsymbol{\chi}}\dot{\boldsymbol{\chi}}^{-1}\boldsymbol{\chi})^{-1}. \tag{S85}$$

Then we are easy to find that

$$\boldsymbol{\Omega}(t)\boldsymbol{\chi} + \boldsymbol{\Gamma}(t)\dot{\boldsymbol{\chi}} = -\ddot{\boldsymbol{\chi}}[(\boldsymbol{\chi} - \dot{\boldsymbol{\chi}}\ddot{\boldsymbol{\chi}}^{-1}\dot{\boldsymbol{\chi}}^{-1})^{-1}\boldsymbol{\chi} + (\dot{\boldsymbol{\chi}} - \ddot{\boldsymbol{\chi}}\dot{\boldsymbol{\chi}}^{-1}\boldsymbol{\chi})^{-1}\dot{\boldsymbol{\chi}}]. \tag{S86}$$

If we rewrite

$$\boldsymbol{\Omega}(t) = (\dddot{\boldsymbol{\chi}} - \ddot{\boldsymbol{\chi}}\dot{\boldsymbol{\chi}}^{-1}\ddot{\boldsymbol{\chi}})(\ddot{\boldsymbol{\chi}} - \dot{\boldsymbol{\chi}}\boldsymbol{\chi}^{-1}\dot{\boldsymbol{\chi}})^{-1}\dot{\boldsymbol{\chi}}\boldsymbol{\chi}^{-1} \tag{S87a}$$

$$\boldsymbol{\Gamma}(t) = -(\dddot{\boldsymbol{\chi}} - \ddot{\boldsymbol{\chi}}\boldsymbol{\chi}^{-1}\dot{\boldsymbol{\chi}})(\ddot{\boldsymbol{\chi}} - \dot{\boldsymbol{\chi}}\boldsymbol{\chi}^{-1}\dot{\boldsymbol{\chi}})^{-1}, \tag{S87b}$$

We can get

$$\boldsymbol{\Omega}(t)\dot{\boldsymbol{\chi}} + \boldsymbol{\Gamma}(t)\ddot{\boldsymbol{\chi}} = -\dddot{\boldsymbol{\chi}} - (\ddot{\boldsymbol{\chi}}\dot{\boldsymbol{\chi}}^{-1}\ddot{\boldsymbol{\chi}})(\ddot{\boldsymbol{\chi}} - \dot{\boldsymbol{\chi}}\boldsymbol{\chi}^{-1}\dot{\boldsymbol{\chi}})^{-1}\dot{\boldsymbol{\chi}}\boldsymbol{\chi}^{-1}\dot{\boldsymbol{\chi}} - (\ddot{\boldsymbol{\chi}}\boldsymbol{\chi}^{-1}\dot{\boldsymbol{\chi}})(\ddot{\boldsymbol{\chi}} - \dot{\boldsymbol{\chi}}\boldsymbol{\chi}^{-1}\dot{\boldsymbol{\chi}})^{-1}\ddot{\boldsymbol{\chi}} \tag{S88}$$

collect them as:

$$\boldsymbol{\Omega}(t)\boldsymbol{\chi} + \boldsymbol{\Gamma}(t)\dot{\boldsymbol{\chi}} = -\ddot{\boldsymbol{\chi}}\big[(\boldsymbol{\chi} - \dot{\boldsymbol{\chi}}\ddot{\boldsymbol{\chi}}^{-1}\dot{\boldsymbol{\chi}}^{-1})^{-1}\boldsymbol{\chi} + (\dot{\boldsymbol{\chi}} - \ddot{\boldsymbol{\chi}}\dot{\boldsymbol{\chi}}^{-1}\boldsymbol{\chi})^{-1}\dot{\boldsymbol{\chi}}\big] \tag{S89a}$$

$$\boldsymbol{\Omega}(t)\dot{\boldsymbol{\chi}} + \boldsymbol{\Gamma}(t)\ddot{\boldsymbol{\chi}} = -\dddot{\boldsymbol{\chi}} - \ddot{\boldsymbol{\chi}}(\boldsymbol{\chi} - \dot{\boldsymbol{\chi}}\ddot{\boldsymbol{\chi}}^{-1}\dot{\boldsymbol{\chi}})^{-1}\dot{\boldsymbol{\chi}} - \ddot{\boldsymbol{\chi}}(\dot{\boldsymbol{\chi}} - \ddot{\boldsymbol{\chi}}\dot{\boldsymbol{\chi}}^{-1}\boldsymbol{\chi})^{-1}\ddot{\boldsymbol{\chi}}. \tag{S89b}$$

Both of them are extermely dirty and tedious, we can use some tricks to make them much simpler, denote

$$\ddot{\boldsymbol{\chi}}\boldsymbol{\chi}^{-1} = \boldsymbol{a} \tag{S90a}$$

$$\dot{\boldsymbol{\chi}}\boldsymbol{\chi}^{-1} = \boldsymbol{b} \tag{S90b}$$

$$\dddot{\boldsymbol{\chi}}\dot{\boldsymbol{\chi}}^{-1} = \boldsymbol{c} \tag{S90c}$$

$$\tag{S90d}$$

to simplify the expression, and we also know

$$\ddot{\boldsymbol{\chi}}\dot{\boldsymbol{\chi}}^{-1} = \ddot{\boldsymbol{\chi}}\boldsymbol{\chi}^{-1}\boldsymbol{\chi}\dot{\boldsymbol{\chi}}^{-1} = \boldsymbol{a}\boldsymbol{b}^{-1} \tag{S91a}$$

$$\boldsymbol{\chi}\dot{\boldsymbol{\chi}}^{-1} = \boldsymbol{b}\boldsymbol{a}^{-1}, \tag{S91b}$$

so that

$$\begin{aligned}
&\boldsymbol{\Omega}(t) + \boldsymbol{\Gamma}(t)\dot{\boldsymbol{\chi}}\boldsymbol{\chi}^{-1} \\
&= -(\boldsymbol{a}^{-1} - \boldsymbol{b}\boldsymbol{a}^{-1}\boldsymbol{b}\boldsymbol{a}^{-1})^{-1} - (\boldsymbol{b}\boldsymbol{a}^{-1} - \boldsymbol{a}\boldsymbol{b}^{-1}\boldsymbol{a}^{-1})^{-1}\boldsymbol{b} \\
&= -\boldsymbol{a} - \boldsymbol{a}[\boldsymbol{b}^{-1}\boldsymbol{a}\boldsymbol{b}^{-1}(\mathbf{I} - \boldsymbol{b}\boldsymbol{a}^{-1}\boldsymbol{b})]^{-1} - \boldsymbol{a}(1 - \boldsymbol{b}^{-1}\boldsymbol{a}\boldsymbol{b}^{-1}) \\
&= -\boldsymbol{a}
\end{aligned} \tag{S92}$$

We have used $(\boldsymbol{A}+\boldsymbol{B})^{-1} \equiv \boldsymbol{A}^{-1} - \boldsymbol{A}^{-1}(\boldsymbol{I} + \boldsymbol{B}\boldsymbol{A}^{-1})^{-1}\boldsymbol{B}\boldsymbol{A}^{-1}$ for arbitray matrics $\boldsymbol{A}$ and $\boldsymbol{B}$, also

$$\begin{aligned}
&\boldsymbol{\Omega}(t) + \boldsymbol{\Gamma}(t)\dot{\boldsymbol{\chi}}\boldsymbol{\chi}^{-1} \\
&= -\boldsymbol{c} - (\boldsymbol{a}^{-1} - \boldsymbol{b}\boldsymbol{a}^{-1}\boldsymbol{b}\boldsymbol{a}^{-1})^{-1} - (\boldsymbol{b}\boldsymbol{a}^{-1} - \boldsymbol{a}\boldsymbol{b}^{-1}\boldsymbol{a}^{-1})\boldsymbol{a}\boldsymbol{b}^{-1} \\
&= -\boldsymbol{c} - \boldsymbol{a}(1 - \boldsymbol{b}\boldsymbol{a}^{-1}\boldsymbol{b})^{-1} - \boldsymbol{a}[\boldsymbol{b}\boldsymbol{a}^{-1}\boldsymbol{b}(1 - \boldsymbol{b}^{-1}\boldsymbol{a}\boldsymbol{b}^{-1})]^{-1} \\
&= -\boldsymbol{c},
\end{aligned} \tag{S93}$$

thus

$$\boldsymbol{\Omega}(t)\boldsymbol{\chi}(t) + \boldsymbol{\Gamma}(t)\dot{\boldsymbol{\chi}}(t) = -\ddot{\boldsymbol{\chi}}(t) \tag{S94a}$$

$$\boldsymbol{\Omega}(t)\dot{\boldsymbol{\chi}}(t) + \boldsymbol{\Gamma}(t)\ddot{\boldsymbol{\chi}}(t) = -\dddot{\boldsymbol{\chi}}(t), \tag{S94b}$$

which is much more simpler.

Our main aim is to move on to find zero-time behaviour of $\boldsymbol{\Omega}(t)$ and $\boldsymbol{\Gamma}(t)$ and get their derivatives. But inverse of matrix is not easy to calculate. So we should consider other ways.

We can obtain following expression by former results,

$$\boldsymbol{\chi}(t) = \boldsymbol{I}t - \frac{1}{3!}\boldsymbol{V}t^3 + \boldsymbol{c}t^5 + o(t^7) \tag{S95a}$$

$$\dot{\boldsymbol{\chi}}(t) = \boldsymbol{I} - \frac{1}{2}\boldsymbol{V}t^2 + 5\boldsymbol{c}t^4 + o(t^6) \tag{S95b}$$

$$\ddot{\boldsymbol{\chi}}(t) = -\boldsymbol{V}t + 20\boldsymbol{c}t^3 + o(t^5) \tag{S95c}$$

$$\dddot{\boldsymbol{\chi}}(t) = -\boldsymbol{V} + 60\boldsymbol{c}t^2 + o(t^2), \tag{S95d}$$

where $\boldsymbol{c} \equiv \frac{1}{5!}\boldsymbol{V}^2 + \sum_\alpha \dot{\boldsymbol{\phi}}_\alpha(0)$ and $o(t^n)$ stands for infinitesimal of order t^n or higher. We know that $(\boldsymbol{A}+\boldsymbol{B})^{-1} \equiv \boldsymbol{A}^{-1} - \boldsymbol{A}^{-1}(\boldsymbol{I}+\boldsymbol{B}\boldsymbol{A}^{-1})^{-1}\boldsymbol{B}\boldsymbol{A}^{-1}$ And for $\boldsymbol{B} = \boldsymbol{\epsilon} =$ infinitesimal we have $(\boldsymbol{A}+\boldsymbol{\epsilon})^{-1} \approx \boldsymbol{A}^{-1} - \boldsymbol{A}^{-1}\boldsymbol{\epsilon}\boldsymbol{A}^{-1}$ So

$$\boldsymbol{\chi}^{-1}(t) = t^{-1} + \frac{1}{6}\boldsymbol{V}t - \boldsymbol{c}t^3 + o(t^5) \tag{S96a}$$

$$\dot{\boldsymbol{\chi}}^{-1}(t) = +\frac{1}{2}\boldsymbol{V}t^2 - 5\boldsymbol{c}t^4 + o(t^6), \tag{S96b}$$

now it is time to get asymptotic expression for what we want, remember the expression for $\boldsymbol{\Omega}(t)$, Eq. (S87a) The first bracket reads:

$$-\boldsymbol{V} + (60\boldsymbol{c} - \boldsymbol{V}^2)t^2 + o(t^4), \tag{S97}$$

inverse of the second bracket:

$$t + \frac{1}{6}t^3 + o(t^5), \tag{S98}$$

so the final result is:

$$\boldsymbol{\Omega}(t) = \big[-\boldsymbol{V} + (60\boldsymbol{c} - \boldsymbol{V}^2)t^2 + o(t^4)\big] \times \big[-\boldsymbol{I}t + \frac{1}{6}t^3 + o(t^5)\big] \times \big[\mathbf{I}t^{-1} - \frac{1}{3}\boldsymbol{V}t + (4\boldsymbol{c} - \frac{1}{12}\boldsymbol{V}^2)t^3 + o(t^5)\big], \tag{S99}$$

we can easily read off that:

$$\boldsymbol{\Omega}(0) = \boldsymbol{V} \tag{S100a}$$

$$\dot{\boldsymbol{\Omega}}(0) = \mathbf{0} \tag{S100b}$$

$$\ddot{\boldsymbol{\Omega}}(0) = -\sum_\alpha \dot{\boldsymbol{\phi}}_\alpha(0) \tag{S100c}$$

Using the same method, note that in Eq. (S87b), first term:

$$\boldsymbol{V}t - (60\boldsymbol{c} + \frac{1}{6}\boldsymbol{V}^2)t^3 + o(t^5), \tag{S101}$$

second term:

$$-\boldsymbol{V}t + (20\boldsymbol{c} + \frac{1}{2}\boldsymbol{V}^2)t^3 + o(t^5), \tag{S102}$$

So we can read off:

$$\boldsymbol{\Gamma}(0) = \mathbf{0} \tag{S103a}$$

$$\dot{\boldsymbol{\Gamma}}(0) = \mathbf{0} \tag{S103b}$$

$$\ddot{\boldsymbol{\Gamma}}(0) = \mathbf{0} \tag{S103c}$$

$$\dddot{\boldsymbol{\Gamma}}(0) = 2\sum_\alpha \dot{\boldsymbol{\phi}}_\alpha(0) \tag{S103d}$$

IV. HEAT CURRENT

A. derivation of heat current

In this section we give the derivation of heat current, first from the definition we have,

$$\hat{J}_\alpha(t) = -\sum_u \hat{Q}_u(t)\dot{\hat{F}}_{\alpha u}(t), \tag{S104}$$

so that

$$
\begin{aligned}
\langle \hat{J}_\alpha(t)\rangle &= -\sum_u \mathrm{tr}_{\mathrm{T}}\left[\hat{Q}_u(t)\dot{\hat{F}}_{\alpha u}(t)\rho_{\mathrm{T}}\right] \\
&= -i\sum_u \mathrm{tr}_{\mathrm{T}}\left\{\hat{Q}_u\big[H_{\mathrm{T}},\hat{F}_{\alpha u}\big]\rho_{\mathrm{T}}(t)\right\} \\
&= -i\sum_u \mathrm{tr}_{\mathrm{T}}\left\{\rho_{\mathrm{T}}(t)\hat{Q}_u\big[H_{\mathrm{T}},\hat{F}_{\alpha u}\big]\right\} \\
&= -i\sum_u \mathrm{tr}_{\mathrm{T}}\left\{\big[\rho_{\mathrm{T}}(t)\hat{Q}_u,H_{\mathrm{T}}\big]\hat{F}_{\alpha u}\right\}
\end{aligned} \tag{S105}
$$

in the bracket

$$
\begin{aligned}
\mathrm{tr}_{\mathrm{T}}\left\{\big[\rho_{\mathrm{T}}(t)\hat{Q}_u,H_{\mathrm{T}}\big]\hat{F}_{\alpha u}\right\} &= \mathrm{tr}_{\mathrm{T}}\left\{\big[\rho_{\mathrm{T}}(t),H_{\mathrm{T}}\big]\hat{Q}_u\hat{F}_{\alpha u}\right\} + \mathrm{tr}_{\mathrm{T}}\left\{\rho_{\mathrm{T}}(t)\big[\hat{Q}_u,H_{\mathrm{T}}\big]\hat{F}_{\alpha u}\right\} \\
&= -i\,\mathrm{tr}_{\mathrm{S}}\left[\hat{Q}_u\,\mathrm{tr}_{\mathrm{B}}(\hat{F}_{\alpha u}\dot{\rho}_{\mathrm{T}}(t))\right] + i\,\mathrm{tr}_{\mathrm{S}}\left[\hat{P}_u\,\mathrm{tr}_{\mathrm{B}}(\hat{F}_{\alpha u}\rho_{\mathrm{T}}(t))\right] \\
&= -i\,\mathrm{tr}_{\mathrm{S}}\left[\hat{Q}_u\dot{\varrho}_{\alpha u}(t)\right] + i\,\mathrm{tr}_{\mathrm{S}}\left[\hat{P}_u\varrho_{\alpha u}(t)\right],
\end{aligned} \tag{S106}
$$

therefore the heat current reads

$$
\langle \hat{J}_\alpha(t)\rangle = -\sum_u \mathrm{tr}_{\mathrm{S}}\left[\hat{Q}_u\dot{\varrho}_{\alpha u}(t)\right] + \sum_u \mathrm{tr}_{\mathrm{S}}\left[\hat{P}_u\varrho_{\alpha u}(t)\right], \tag{S107}
$$

where

$$
\varrho_{\alpha u}(t) = \sum_v \left[\Omega_{\alpha uv}(t)\hat{Q}_v^{\oplus} + \Gamma_{\alpha uv}(t)\hat{P}_v^{\oplus} + \gamma_{\alpha uv}(t)\hat{Q}_v^{\ominus} - \gamma'_{\alpha uv}(t)\hat{P}_v^{\ominus}\right]\rho_{\mathrm{S}}(t). \tag{S108}
$$

The first term in Eq. (S107) is more complex so we firstly deal with the second term.

$$
\begin{aligned}
&\mathrm{tr}_{\mathrm{S}}\left[\hat{P}_u\varrho_{\alpha u}(t)\right] \\
=\ &\mathrm{tr}_{\mathrm{S}}\left\{\hat{P}_u\sum_v\left[\Omega_{\alpha uv}(t)\hat{Q}_v^{\oplus} + \Gamma_{\alpha uv}(t)\hat{P}_v^{\oplus} + \gamma_{\alpha uv}(t)\hat{Q}_v^{\ominus} - \gamma'_{\alpha uv}(t)\hat{P}_v^{\ominus}\right]\rho_{\mathrm{S}}(t)\right\} \\
=\ &\sum_v\left\{\Omega_{\alpha uv}(t)\,\mathrm{tr}_{\mathrm{S}}\left[\hat{P}_u\hat{Q}_v^{\oplus}\rho_{\mathrm{S}}(t)\right] + \Gamma_{\alpha uv}(t)\,\mathrm{tr}_{\mathrm{S}}\left[\hat{P}_u\hat{P}_v^{\oplus}\rho_{\mathrm{S}}(t)\right] + \gamma_{\alpha uv}(t)\,\mathrm{tr}_{\mathrm{S}}\left[\hat{P}_u\hat{Q}_v^{\ominus}\rho_{\mathrm{S}}(t)\right]\right\} \\
=\ &\sum_v\left\{\Omega_{\alpha uv}(t)\frac{1}{2}\big\langle\{\hat{P}_u(t),\hat{Q}_v(t)\}\big\rangle + \Gamma_{\alpha uv}(t)\frac{1}{2}\big\langle\{\hat{P}_u(t),\hat{P}_v(t)\}\big\rangle - i\gamma_{\alpha uv}(t)\big\langle[\hat{P}_u(t),\hat{Q}_v(t)]\big\rangle\right\} \\
=\ &\sum_v\Omega_{\alpha uv}(t)\big[W_{uv}^{PQ}(t) + P_u(t)Q_v(t)\big] + \sum_v\Gamma_{\alpha uv}(t)\big[W_{uv}^{PP}(t) + P_u(t)P_v(t)\big] - \sum_v\gamma_{\alpha uv}(t)\delta_{uv},
\end{aligned} \tag{S109}
$$

so the second term gives us

$$
\sum_{uv}\Omega_{\alpha uv}(t)\big[W_{uv}^{PQ}(t) + P_u(t)Q_v(t)\big] + \sum_{uv}\Gamma_{\alpha uv}(t)\big[W_{uv}^{PP}(t) + P_u(t)P_v(t)\big] - \sum_u\gamma_{\alpha uu}(t). \tag{S110}
$$

It is difficult to directly give expression of the first term in Eq. (S107). Let's use a simple trick, denote

$$
H_\alpha(t) \equiv -\int_0^t d\tau\sum_u \mathrm{tr}_{\mathrm{S}}\left[\hat{Q}_u\dot{\varrho}_{\alpha u}(\tau)\right] = -\sum_u \mathrm{tr}_{\mathrm{S}}\left[\hat{Q}_u\varrho_{\alpha u}(t)\right] + \text{constant}, \tag{S111}
$$

once we obtain $H_\alpha(t)$ we can take derivative of it to get $J_\alpha(t)$. Put Eq. (S108) into Eq. (S111) we can obtain

$$
\begin{aligned}
H_\alpha(t) &= -\sum_u \mathrm{tr}_{\mathrm{S}}\left\{\hat{Q}_u\sum_v\left[\Omega_{\alpha uv}(t)\hat{Q}_v^{\oplus} + \Gamma_{\alpha uv}(t)\hat{P}_v^{\oplus} + \gamma_{\alpha uv}(t)\hat{Q}_v^{\ominus} - \gamma'_{\alpha uv}(t)\hat{P}_v^{\ominus}\right]\rho_{\mathrm{S}}(t)\right\} \\
&= -\sum_{uv}\left[\Omega_{\alpha uv}(t)\frac{1}{2}\big\langle\{\hat{Q}_u(t),\hat{Q}_v(t)\}\big\rangle + \Gamma_{\alpha uv}(t)\frac{1}{2}\big\langle\{\hat{Q}_u(t),\hat{P}_v(t)\}\big\rangle + i\gamma'_{\alpha uv}(t)\big\langle[\hat{Q}_u(t),\hat{P}_v(t)]\big\rangle\right] \\
&= -\sum_{uv}\left[\Omega_{\alpha uv}(t)\frac{1}{2}\big\langle\{\hat{Q}_u(t),\hat{Q}_v(t)\}\big\rangle + \Gamma_{\alpha uv}(t)\frac{1}{2}\big\langle\{\hat{Q}_u(t),\hat{P}_v(t)\}\big\rangle\right] + \sum_u\gamma'_{\alpha uu}(t),
\end{aligned} \tag{S112}
$$

we can express $H_\alpha(t)$ in terms of first and second order moment functions

$$H_\alpha(t) = -\sum_{uv}\left\{\Omega_{\alpha uv}(t)\big[W^{QQ}_{uv}(t) + Q_u(t)Q_v(t)\big] + \Gamma_{\alpha uv}(t)[W^{QP}_{uv}(t) + Q_u(t)P_v(t)]\right\} + \sum_u \gamma'_{\alpha uu}(t), \tag{S113}$$

thus the

$$\big\langle \hat{J}_\alpha(t)\big\rangle = \frac{dH_\alpha(t)}{dt} + \sum_{uv}\Omega_{\alpha uv}(t)\big[W^{PQ}_{uv}(t) + P_u(t)Q_v(t)\big] + \sum_{uv}\Gamma_{\alpha uv}(t)\big[W^{PP}_{uv}(t) + P_u(t)P_v(t)\big] - \sum_u \gamma_{\alpha uu}(t). \tag{S114}$$

B. analysis of nonequilibrium steady state

First we give expression of heat current at nonequilibrium steady state, which means we take the limit as t goes to infinity. The first term in Eq. (S114) will vanish. Since from Eq. (S10) we know $Q_u(\infty) = 0$ and $P_u(\infty) = 0$, in nonequilibrium steady state Eq. (S114) reduces to

$$\begin{aligned}\big\langle \hat{J}_\alpha(\infty)\big\rangle &= \sum_{uv}\Omega_{\alpha uv}(\infty)W^{QP}_{uv}(\infty) + \sum_{uv}\Gamma_{\alpha uv}(\infty)W^{PP}_{uv}(\infty) - \sum_u \gamma_{\alpha uu}(\infty)\\ &= \mathrm{tr}\left[\boldsymbol{\Omega}_\alpha(\infty)\boldsymbol{W}^{QP}(\infty)\right] + \mathrm{tr}\left[\boldsymbol{\Gamma}_\alpha(\infty)\boldsymbol{W}^{PP}(\infty)\right] - \mathrm{tr}\left[\boldsymbol{\gamma}_\alpha(\infty)\right]\end{aligned} \tag{S115}$$

to further simplify and analyze this result, we introduce covariance matrix as

$$\boldsymbol{W}(t) \equiv \begin{bmatrix}\boldsymbol{W}^{QQ}(t) & \boldsymbol{W}^{QP}(t)\\ \boldsymbol{W}^{PQ}(t) & \boldsymbol{W}^{PP}(t)\end{bmatrix} = \frac{1}{2}\left\langle\left\{\begin{bmatrix}\delta\hat{\boldsymbol{Q}}(t)\\ \delta\hat{\boldsymbol{P}}(t)\end{bmatrix}, \begin{bmatrix}\delta\hat{\boldsymbol{Q}}(t)\\ \delta\hat{\boldsymbol{P}}(t)\end{bmatrix}^{\mathrm{T}}\right\}\right\rangle, \tag{S116}$$

with

$$\boldsymbol{W}^{PQ}(t) \equiv \left[\boldsymbol{W}^{QP}(t)\right]^{\mathrm{T}}, \tag{S117}$$

and from Eq. (8) in the main text we get

$$\begin{bmatrix}\delta\dot{\hat{\boldsymbol{Q}}}(t)\\ \delta\dot{\hat{\boldsymbol{P}}}(t)\end{bmatrix} = \boldsymbol{\Lambda}(t)\begin{bmatrix}\delta\hat{\boldsymbol{Q}}(t)\\ \delta\hat{\boldsymbol{P}}(t)\end{bmatrix} + \sum_\alpha \begin{bmatrix}0\\ \hat{\boldsymbol{F}}^{\mathrm{eff}}_\alpha(t)\end{bmatrix}. \tag{S118}$$

Take derivative of both side of Eq. (S116) to get EOM for $\boldsymbol{W}(t)$ matrix.

$$\begin{aligned}\dot{\boldsymbol{W}}(t) &= \frac{1}{2}\left\langle\left\{\begin{bmatrix}\delta\dot{\hat{\boldsymbol{Q}}}(t)\\ \delta\dot{\hat{\boldsymbol{P}}}(t)\end{bmatrix}, \begin{bmatrix}\delta\hat{\boldsymbol{Q}}(t)\\ \delta\hat{\boldsymbol{P}}(t)\end{bmatrix}^{\mathrm{T}}\right\}\right\rangle + \frac{1}{2}\left\langle\left\{\begin{bmatrix}\delta\hat{\boldsymbol{Q}}(t)\\ \delta\hat{\boldsymbol{P}}(t)\end{bmatrix}, \begin{bmatrix}\delta\dot{\hat{\boldsymbol{Q}}}(t)\\ \delta\dot{\hat{\boldsymbol{P}}}(t)\end{bmatrix}^{\mathrm{T}}\right\}\right\rangle\\
&= \frac{1}{2}\boldsymbol{\Lambda}(t)\left\langle\left\{\begin{bmatrix}\delta\hat{\boldsymbol{Q}}(t)\\ \delta\hat{\boldsymbol{P}}(t)\end{bmatrix}, \begin{bmatrix}\delta\hat{\boldsymbol{Q}}(t)\\ \delta\hat{\boldsymbol{P}}(t)\end{bmatrix}^{\mathrm{T}}\right\}\right\rangle + \frac{1}{2}\sum_\alpha\left\langle\left\{\begin{bmatrix}0\\ \hat{\boldsymbol{F}}^{\mathrm{eff}}_\alpha(t)\end{bmatrix}, \begin{bmatrix}\delta\hat{\boldsymbol{Q}}(t)\\ \delta\hat{\boldsymbol{P}}(t)\end{bmatrix}^{\mathrm{T}}\right\}\right\rangle\\
&\quad + \frac{1}{2}\left\langle\left\{\begin{bmatrix}\delta\hat{\boldsymbol{Q}}(t)\\ \delta\hat{\boldsymbol{P}}(t)\end{bmatrix}, \begin{bmatrix}\delta\hat{\boldsymbol{Q}}(t)\\ \delta\hat{\boldsymbol{P}}(t)\end{bmatrix}^{\mathrm{T}}\right\}\right\rangle\boldsymbol{\Lambda}^{\mathrm{T}}(t) + \frac{1}{2}\sum_\alpha\left\langle\left\{\begin{bmatrix}\delta\hat{\boldsymbol{Q}}(t)\\ \delta\hat{\boldsymbol{P}}(t)\end{bmatrix}, \begin{bmatrix}0\\ \hat{\boldsymbol{F}}^{\mathrm{eff}}_\alpha(t)\end{bmatrix}^{\mathrm{T}}\right\}\right\rangle\\
&= \boldsymbol{\Lambda}(t)\boldsymbol{W}(t) + \boldsymbol{W}(t)\boldsymbol{\Lambda}^{\mathrm{T}}(t)\\
&\quad + \frac{1}{2}\left\langle\begin{bmatrix}0 & 0\\ \{\hat{\boldsymbol{F}}^{\mathrm{eff}}_\alpha(t), \delta\hat{\boldsymbol{Q}}^{\mathrm{T}}(t)\} & \{\hat{\boldsymbol{F}}^{\mathrm{eff}}_\alpha(t), \delta\hat{\boldsymbol{P}}^{\mathrm{T}}(t)\}\end{bmatrix}\right\rangle + \frac{1}{2}\left\langle\begin{bmatrix}0 & \{\delta\hat{\boldsymbol{Q}}(t), \big[\hat{\boldsymbol{F}}^{\mathrm{eff}}_\alpha(t)\big]^{\mathrm{T}}\}\\ 0 & \{\delta\hat{\boldsymbol{P}}(t), \big[\hat{\boldsymbol{F}}^{\mathrm{eff}}_\alpha(t)\big]^{\mathrm{T}}\}\end{bmatrix}\right\rangle,\end{aligned} \tag{S119}$$

note that

$$\frac{1}{2}\big\langle\{\hat{\boldsymbol{F}}^{\mathrm{eff}}_\alpha(t), \delta\hat{\boldsymbol{Q}}^{\mathrm{T}}(t)\}\big\rangle = \mathrm{Re}\left[\hat{\boldsymbol{F}}^{\mathrm{eff}}_\alpha(t)\delta\hat{\boldsymbol{Q}}^{\mathrm{T}}(t)\right] = \mathrm{Re}\left[\hat{\boldsymbol{F}}^{\mathrm{eff}}_\alpha(t)\hat{\boldsymbol{Q}}^{\mathrm{T}}(t)\right] = \boldsymbol{\gamma}'_\alpha(t), \tag{S120}$$

following this trick we can rewrite Eq. (S119) as

$$\dot{\boldsymbol{W}}(t) = \boldsymbol{\Lambda}(t)\boldsymbol{W}(t) + \boldsymbol{W}(t)\boldsymbol{\Lambda}^{\mathrm{T}}(t) + \sum_\alpha \boldsymbol{U}_\alpha(t), \tag{S121}$$

where

$$\boldsymbol{U}_\alpha(t) = \begin{bmatrix}0 & \big[\boldsymbol{\gamma}'_\alpha(t)\big]^{\mathrm{T}}\\ \boldsymbol{\gamma}'_\alpha(t) & \boldsymbol{\gamma}_\alpha(t) + \big[\boldsymbol{\gamma}_\alpha(t)\big]^{\mathrm{T}}\end{bmatrix}, \tag{S122}$$

take the limit with t tending to infinity of both sides of Eq. (S121) we obtain

$$\boldsymbol{\Lambda}(\infty)\boldsymbol{W}(\infty)+\boldsymbol{W}(\infty)\boldsymbol{\Lambda}^{\mathrm{T}}(\infty)+\sum_\alpha \boldsymbol{U}_\alpha(\infty)=\mathbf{0}, \tag{S123}$$

with Eq. (S116) we can get useful relations at nonequilibrium steady state

$$\boldsymbol{W}^{PQ}(\infty)+\boldsymbol{W}^{QP}(\infty)=\mathbf{0} \tag{S124a}$$

$$\sum_\alpha \boldsymbol{\gamma}'_\alpha(\infty)=-\boldsymbol{W}^{PP}(\infty)+\boldsymbol{\Omega}(\infty)\boldsymbol{W}^{QQ}(\infty)+\boldsymbol{\Gamma}(t)\boldsymbol{W}^{PQ}(\infty) \tag{S124b}$$

$$\sum_\alpha\Big(\boldsymbol{\gamma}_\alpha(\infty)+\big[\boldsymbol{\gamma}_\alpha(\infty)\big]^{\mathrm{T}}\Big)=\boldsymbol{\Omega}(\infty)\boldsymbol{W}^{QP}(\infty)+\boldsymbol{W}^{PQ}(\infty)\boldsymbol{\Omega}(\infty)+\boldsymbol{\Gamma}(\infty)\boldsymbol{W}^{PP}(\infty)+\boldsymbol{W}^{PP}(\infty)\boldsymbol{\Gamma}(\infty), \tag{S124c}$$

take the trace of both sides of Eq. (S124c) we get

$$\sum_\alpha \mathrm{tr}\left[\boldsymbol{\gamma}_\alpha(\infty)\right]=\mathrm{tr}\left[\boldsymbol{\Gamma}(\infty)\boldsymbol{W}^{PP}(\infty)\right], \tag{S125}$$

note that from Eq. (S117) and Eq. (S124a) we know both $\boldsymbol{W}^{PQ}(\infty)$ and $\boldsymbol{W}^{QP}(\infty)$ are antisymmetric matrix. With $\boldsymbol{\Omega}_\alpha(t)$ being symmetric we know $\mathrm{tr}\left[\boldsymbol{\Omega}_\alpha(\infty)\boldsymbol{W}^{QP}(\infty)\right]=0$. Therefore Eq. (S115) can be simplified as

$$\left\langle \hat{J}^{\mathrm{st}}_\alpha\right\rangle=\mathrm{tr}\left[\boldsymbol{\Gamma}_\alpha(\infty)\boldsymbol{W}^{PP}(\infty)\right]-\mathrm{tr}\left[\boldsymbol{\gamma}_\alpha(\infty)\right] \tag{S126}$$

From Eq. (S125) and Eq. (S49) we directly derive the conservation law of current,

$$\sum_\alpha\left\langle \hat{J}^{\mathrm{st}}_\alpha\right\rangle=0 \tag{S127}$$

C. analysis of equilibrium state

When the system is coupled with two reservoirs at the same temperature, namely

$$\beta_\alpha=\beta \quad \text{for } \alpha=1,2 \tag{S128}$$

they will fall into equilibrium state. In the former theoretical derivation basen on EOM of $\boldsymbol{W}(t)$, we have no chance to introduce the condition Eq. (S128). Here we will directly use Eq. (S44) to conduct asymptotic analysis of $\boldsymbol{\gamma_\alpha}$ and $\boldsymbol{\gamma'_\alpha}$ at equilibrium state with the help of fluctuation-dissipation theoremEq. (S40):

First we consider

$$\begin{aligned}
k^{00}_{\alpha vw}(t)&=T^{00}_{\alpha vw}(t)\\
&=\sum_{u_1v_1}\int_0^t \mathrm{d}\tau_1\int_0^t \mathrm{d}\tau_2\,\chi_{vu_1}(\tau_1)a_{\alpha v_1u_1}(\tau_1-\tau_2)\chi_{wv_1}(\tau_2)\\
&=\mathrm{Re}\sum_{u_1v_1}\int_0^t \mathrm{d}\tau_1\int_0^t \mathrm{d}\tau_2\,\chi_{vu_1}(\tau_1)c_{\alpha v_1u_1}(\tau_1-\tau_2)\chi_{wv_1}(\tau_2)\\
&=\mathrm{Re}\,\frac{1}{\pi}\sum_{u_1v_1}\int_0^t \mathrm{d}\tau_1\int_0^t \mathrm{d}\tau_2\,\chi_{vu_1}(\tau_1)\int_{-\infty}^{\infty}\mathrm{d}\omega\, e^{-i\omega(\tau_1-\tau_2)}\frac{\tilde{\phi}^{(-)}_{\alpha v_1u_1}(\omega)}{1-e^{-\beta\omega_\alpha}}\chi_{wv_1}(\tau_2)\\
&=\mathrm{Re}\,\frac{1}{\pi}\sum_{u_1v_1}\int_{-\infty}^{\infty}\mathrm{d}\omega\,\frac{\tilde{\phi}^{(-)}_{\alpha v_1u_1}(\omega)}{1-e^{-\beta\omega_\alpha}}\left(\int_0^t \mathrm{d}\tau_1\,\chi_{vu_1}(\tau_1)e^{-i\omega\tau_1}\right)\left(\int_0^t \mathrm{d}\tau_2\,\chi_{wv_1}(\tau_2)e^{i\omega\tau_2}\right),
\end{aligned} \tag{S129}$$

therefore

$$k^{00}_{\alpha vw}(\infty)=\sum_{u_1v_1}\frac{1}{\pi}\,\mathrm{Re}\int_{-\infty}^{\infty}\mathrm{d}\omega\,\frac{\tilde{\phi}^{(-)}_{\alpha v_1u_1}(\omega)}{1-e^{-\beta\omega_\alpha}}\chi^*_{vu_1}(\omega)\chi_{wv_1}(\omega). \tag{S130}$$

Note that

$$\boldsymbol{\chi}(\omega)=\Big[\boldsymbol{V}-\sum_\alpha\tilde{\boldsymbol{\phi}}_\alpha(\omega)-\omega\mathbf{I}\Big]^{-1}, \tag{S131}$$

we have

$$\begin{aligned}
2i\boldsymbol{\chi}^{(-)}(\omega) &= \boldsymbol{\chi}(\omega) - \boldsymbol{\chi}^{\dagger}(\omega) \\
&= \big[\boldsymbol{V} - \sum_{\alpha} \tilde{\boldsymbol{\phi}}_{\alpha}(\omega) - \omega\mathbf{I}\big]^{-1} - \big[\boldsymbol{V} - \sum_{\alpha} \tilde{\boldsymbol{\phi}}^{\dagger}_{\alpha}(\omega) - \omega\mathbf{I}\big]^{-1} \\
&= \big[\boldsymbol{V} - \sum_{\alpha} \tilde{\boldsymbol{\phi}}_{\alpha}(\omega) - \omega\mathbf{I}\big]^{-1} \Big[\Big(\boldsymbol{V} - \sum_{\alpha} \tilde{\boldsymbol{\phi}}^{\dagger}_{\alpha}(\omega) - \omega\mathbf{I}\Big) - \Big(\boldsymbol{V} - \sum_{\alpha} \tilde{\boldsymbol{\phi}}_{\alpha}(\omega) - \omega\mathbf{I}\Big)\Big] \big[\boldsymbol{V} - \sum_{\alpha} \tilde{\boldsymbol{\phi}}^{\dagger}_{\alpha}(\omega) - \omega\mathbf{I}\big]^{-1} \\
&= \big[\boldsymbol{V} - \sum_{\alpha} \tilde{\boldsymbol{\phi}}_{\alpha}(\omega) - \omega\mathbf{I}\big]^{-1} \big[\sum_{\alpha} \tilde{\boldsymbol{\phi}}_{\alpha}(\omega) - \sum_{\alpha} \tilde{\boldsymbol{\phi}}^{\dagger}_{\alpha}(\omega)\big] \big[\boldsymbol{V} - \sum_{\alpha} \tilde{\boldsymbol{\phi}}^{\dagger}_{\alpha}(\omega) - \omega\mathbf{I}\big]^{-1},
\end{aligned} \tag{S132}$$

thus

$$\boldsymbol{\chi}^{(-)}(\omega) = \sum_{\alpha} \boldsymbol{\chi}(\omega)\tilde{\boldsymbol{\phi}}^{(-)}_{\alpha}(\omega)\boldsymbol{\chi}^{\dagger}(\omega) \tag{S133}$$

put Eq. (S133) into Eq. (S130) and apply conditionEq. (S128) we obtain

$$\sum_{\alpha} k^{00}_{\alpha v w}(\infty) = \frac{1}{\pi} \operatorname{Re} \int_{-\infty}^{\infty} \mathrm{d}\omega\, \frac{\chi^{(-)}_{wv}(\omega)}{1 - e^{-\beta\omega}} = \frac{1}{\pi} \operatorname{Re} \int_{-\infty}^{\infty} \mathrm{d}\omega\, C^{(+)}_{wv}(\omega) = \operatorname{Re} C_{wv}(0) = W^{QQ}_{wv}(\mathrm{eq}), \tag{S134}$$

with $C_{wv}(t)$ being the correlation function of the system. Following the same trick, we turn to

$$\begin{aligned}
k^{01}_{\alpha v w}(t) &= T^{01}_{\alpha v w}(t) \\
&= \sum_{u_1 v_1} \int_0^t \mathrm{d}\tau_1 \int_0^t \mathrm{d}\tau_2\, \chi_{v u_1}(\tau_1) a_{\alpha v_1 u_1}(\tau_1 - \tau_2) \dot{\chi}_{w v_1}(\tau_2) \\
&= \operatorname{Re} \sum_{u_1 v_1} \int_0^t \mathrm{d}\tau_1 \int_0^t \mathrm{d}\tau_2\, \chi_{v u_1}(\tau_1) c_{\alpha v_1 u_1}(\tau_1 - \tau_2) \dot{\chi}_{w v_1}(\tau_2) \\
&= \operatorname{Re} \frac{1}{\pi} \sum_{u_1 v_1} \int_0^t \mathrm{d}\tau_1 \int_0^t \mathrm{d}\tau_2\, \chi_{v u_1}(\tau_1) \int_{-\infty}^{\infty} \mathrm{d}\omega\, e^{-i\omega(\tau_1 - \tau_2)} \frac{\tilde{\phi}^{(-)}_{\alpha v_1 u_1}(\omega)}{1 - e^{-\beta\omega_\alpha}} \dot{\chi}_{w v_1}(\tau_2) \\
&= \operatorname{Re} \frac{1}{\pi} \sum_{u_1 v_1} \int_{-\infty}^{\infty} \mathrm{d}\omega\, \frac{\tilde{\phi}^{(-)}_{\alpha v_1 u_1}(\omega)}{1 - e^{-\beta\omega_\alpha}} \Big(\int_0^t \mathrm{d}\tau_1\, \chi_{v u_1}(\tau_1) e^{-i\omega\tau_1}\Big)\Big(\int_0^t \mathrm{d}\tau_2\, \dot{\chi}_{w v_1}(\tau_2) e^{i\omega\tau_2}\Big),
\end{aligned} \tag{S135}$$

since

$$\int_0^{\infty} \mathrm{d}\tau_2\, \dot{\chi}_{w v_1}(\tau_2) e^{i\omega\tau_2} = -i\omega \int_0^{\infty} \mathrm{d}\tau_2\, \chi_{w v_1}(\tau_2) e^{i\omega\tau_2} = -i\omega\chi_{w v_1}(\omega), \tag{S136}$$

we have

$$k^{01}_{\alpha v w}(\infty) = \sum_{u_1 v_1} \frac{1}{\pi} \operatorname{Re} \int_{-\infty}^{\infty} \mathrm{d}\omega\, -i\omega \frac{\tilde{\phi}^{(-)}_{\alpha v_1 u_1}(\omega)}{1 - e^{-\beta_\alpha\omega}} \chi^{*}_{v u_1}(\omega)\chi_{w v_1}(\omega) = \sum_{u_1 v_1} \frac{1}{\pi} \operatorname{Im} \int_{-\infty}^{\infty} \mathrm{d}\omega\, \omega \frac{\tilde{\phi}^{(-)}_{\alpha v_1 u_1}(\omega)}{1 - e^{-\beta_\alpha\omega}} \chi^{*}_{v u_1}(\omega)\chi_{w v_1}(\omega), \tag{S137}$$

however

$$\sum_{\alpha} k^{01}_{\alpha v w}(\infty) = \frac{1}{\pi} \operatorname{Re} \int_{-\infty}^{\infty} \mathrm{d}\omega\, \frac{-i\omega\chi^{(-)}_{wv}(\omega)}{1 - e^{-\beta\omega}} = \frac{1}{\pi} \operatorname{Im} \int_{-\infty}^{\infty} \mathrm{d}\omega\, \frac{\omega\chi^{(-)}_{wv}(\omega)}{1 - e^{-\beta\omega}} = 0, \tag{S138}$$

further

$$\begin{aligned}
k^{02}_{\alpha vw}(t) &= T^{02}_{\alpha vw}(t) + \sum_{u_1}\int_0^t \mathrm{d}\tau\, \chi_{vu_1}(\tau)a_{\alpha u_1 w}(\tau) \\
&= \sum_{u_1 v_1}\int_0^t \mathrm{d}\tau_1 \int_0^t \mathrm{d}\tau_2\, \chi_{vu_1}(\tau_1)a_{\alpha v_1 u_1}(\tau_1-\tau_2)\ddot{\chi}_{wv_1}(\tau_2) + \sum_{u_1}\int_0^t \mathrm{d}\tau\, \chi_{vu_1}(\tau)a_{\alpha u_1 w}(\tau) \\
&= \mathrm{Re}\sum_{u_1 v_1}\int_0^t \mathrm{d}\tau_1 \int_0^t \mathrm{d}\tau_2\, \chi_{vu_1}(\tau_1)c_{\alpha v_1 u_1}(\tau_1-\tau_2)\ddot{\chi}_{wv_1}(\tau_2) + \sum_{u_1}\int_0^t \mathrm{d}\tau\, \chi_{vu_1}(\tau)a_{\alpha u_1 w}(\tau) \\
&= \mathrm{Re}\,\frac{1}{\pi}\sum_{u_1 v_1}\int_0^t \mathrm{d}\tau_1 \int_0^t \mathrm{d}\tau_2\, \chi_{vu_1}(\tau_1)\int_{-\infty}^{\infty}\mathrm{d}\omega\, e^{-i\omega(\tau_1-\tau_2)}\frac{\tilde{\phi}^{(-)}_{\alpha v_1 u_1}(\omega)}{1-e^{-\beta\omega_\alpha}}\ddot{\chi}_{wv_1}(\tau_2) + \sum_{u_1}\int_0^t \mathrm{d}\tau\, \chi_{vu_1}(\tau)a_{\alpha u_1 w}(\tau) \\
&= \mathrm{Re}\,\frac{1}{\pi}\sum_{u_1 v_1}\int_{-\infty}^{\infty}\mathrm{d}\omega\, \frac{\tilde{\phi}^{(-)}_{\alpha v_1 u_1}(\omega)}{1-e^{-\beta\omega_\alpha}}\left(\int_0^t \mathrm{d}\tau_1\, \chi_{vu_1}(\tau_1)e^{-i\omega\tau_1}\right)\left(\int_0^t \mathrm{d}\tau_2\, \ddot{\chi}_{wv_1}(\tau_2)e^{i\omega\tau_2}\right) + \sum_{u_1}\int_0^t \mathrm{d}\tau\, \chi_{vu_1}(\tau)a_{\alpha u_1 w}(\tau),
\end{aligned} \tag{S139}$$

$$\int_0^\infty \mathrm{d}\tau_2\, \ddot{\chi}_{wv_1}(\tau_2)e^{i\omega\tau_2} = -\omega^2\int_0^\infty \mathrm{d}\tau_2\, \chi_{wv_1}(\tau_2)e^{i\omega\tau_2} - \delta_{wv_1} = -\omega^2\chi_{wv_1}(\omega) - \delta_{wv_1}, \tag{S140}$$

substitude into Eq. (S139) we arrive at

$$k^{02}_{\alpha vw}(\infty) = -\sum_{u_1 v_1}\frac{1}{\pi}\,\mathrm{Re}\int_{-\infty}^{\infty}\mathrm{d}\omega\, \omega^2\frac{\tilde{\phi}^{(-)}_{\alpha v_1 u_1}(\omega)}{1-e^{-\beta\omega_\alpha}}\chi^*_{vu_1}(\omega)\chi_{wv_1}(\omega), \tag{S141}$$

therefore

$$\sum_\alpha k^{02}_{\alpha vw}(\infty) = -\frac{1}{\pi}\,\mathrm{Re}\int_{-\infty}^{\infty}\mathrm{d}\omega\, \omega^2\frac{\chi^{(-)}_{wv}(\omega)}{1-e^{-\beta\omega}} = -\frac{1}{\pi}\,\mathrm{Re}\int_{-\infty}^{\infty}\mathrm{d}\omega\, \frac{\omega^2\chi^{(-)}_{wv}(\omega)}{1-e^{-\beta\omega}} = -\frac{1}{\pi}\,\mathrm{Re}\int_{-\infty}^{\infty}\mathrm{d}\omega\, \frac{\left[\chi^{PP}_{wv}(\omega)\right]^{(-)}}{1-e^{-\beta\omega}} = -W^{PP}_{wv}(\mathrm{eq}), \tag{S142}$$

put Eq. (S134), Eq. (S138) and Eq. (S142) into Eq. (S44) we obtain

$$\sum_\alpha \gamma'_{\alpha uv}(\mathrm{eq}) = \sum_w \left[\Omega_{uw}(\infty)W^{QQ}_{wv}(\mathrm{eq})\right] - W^{PP}_{uv}(\mathrm{eq}), \tag{S143}$$

comparing Eq. (S143) with Eq. (S124b) we notice that $\boldsymbol{W}^{PQ}(\mathrm{eq})$ will not contribute. Here we can prove that $\boldsymbol{W}^{PQ}(\mathrm{eq}) = \mathbf{0}$, from FDT we know

$$W^{PQ}_{uv}(\mathrm{eq}) = \frac{1}{\pi}\,\mathrm{Re}\int_{-\infty}^{\infty}\mathrm{d}\omega\, \frac{\left[\chi^{PQ}_{wv}(\omega)\right]^{(-)}}{1-e^{-\beta\omega}}, \tag{S144}$$

since

$$\boldsymbol{\chi}^{(-)}_{PQ}(\omega) = \frac{\boldsymbol{\chi}_{PQ}(\omega) - \boldsymbol{\chi}^\dagger_{PQ}(\omega)}{2i} = \frac{-i\omega\boldsymbol{\chi}(\omega) - \big(-i\omega\boldsymbol{\chi}(\omega)\big)^\dagger}{2i} = -\omega\boldsymbol{\chi}^{(+)}(\omega), \tag{S145}$$

is symmetric, $W^{PQ}_{uv}(\mathrm{eq})$ is symmetric as well. But from EOM of $\boldsymbol{W}(t)$ we know $W^{PQ}_{uv}(\mathrm{eq})$ should be anti-symmetric. Therefore we know

$$\boldsymbol{W}^{PQ}(\mathrm{eq}) = \mathbf{0}. \tag{S146}$$

Repeat the same process to $k^{10}_{\alpha vw}(t), k^{11}_{\alpha vw}(t)$ and $k^{12}_{\alpha vw}(t)$, we summarize the results below

$$k^{10}_{\alpha vw}(\infty) = -\sum_{u_1 v_1}\frac{1}{\pi}\,\mathrm{Im}\int_{-\infty}^{\infty}\mathrm{d}\omega\, \omega\frac{\tilde{\phi}^{(-)}_{\alpha v_1 u_1}(\omega)}{1-e^{-\beta_\alpha\omega}}\chi^*_{vu_1}(\omega)\chi_{wv_1}(\omega) \tag{S147a}$$

$$k^{11}_{\alpha vw}(\infty) = \sum_{u_1 v_1}\frac{1}{\pi}\,\mathrm{Re}\int_{-\infty}^{\infty}\mathrm{d}\omega\, \omega^2\frac{\tilde{\phi}^{(-)}_{\alpha v_1 u_1}(\omega)}{1-e^{-\beta_\alpha\omega}}\chi^*_{vu_1}(\omega)\chi_{wv_1}(\omega) \tag{S147b}$$

$$k^{12}_{\alpha vw}(\infty) = \sum_{u_1 v_1}\frac{1}{\pi}\,\mathrm{Im}\int_{-\infty}^{\infty}\mathrm{d}\omega\, \omega^3\frac{\tilde{\phi}^{(-)}_{\alpha v_1 u_1}(\omega)}{1-e^{-\beta_\alpha\omega}}\chi^*_{vu_1}(\omega)\chi_{wv_1}(\omega), \tag{S147c}$$

similarly,

$$\sum_{\alpha} k^{10}_{\alpha vw}(\infty) = \sum_{\alpha} k^{12}_{\alpha vw}(\infty) = 0, \tag{S148}$$

for $k^{11}_{\alpha vw}(\infty)$ we show the process

$$\begin{aligned}
k^{11}_{\alpha vw}(t) &= T^{11}_{\alpha vw}(t) \\
&= \sum_{u_1 v_1} \int_0^t \mathrm{d}\tau_1 \int_0^t \mathrm{d}\tau_2\, \dot{\chi}_{vu_1}(\tau_1) a_{\alpha v_1 u_1}(\tau_1 - \tau_2) \dot{\chi}_{wv_1}(\tau_2) \\
&= \mathrm{Re} \sum_{u_1 v_1} \int_0^t \mathrm{d}\tau_1 \int_0^t \mathrm{d}\tau_2\, \dot{\chi}_{vu_1}(\tau_1) c_{\alpha v_1 u_1}(\tau_1 - \tau_2) \dot{\chi}_{wv_1}(\tau_2) \\
&= \mathrm{Re}\, \frac{1}{\pi} \sum_{u_1 v_1} \int_0^t \mathrm{d}\tau_1 \int_0^t \mathrm{d}\tau_2\, \dot{\chi}_{vu_1}(\tau_1) \int_{-\infty}^{\infty} \mathrm{d}\omega\, e^{-i\omega(\tau_1 - \tau_2)} \frac{\tilde{\phi}^{(-)}_{\alpha v_1 u_1}(\omega)}{1 - e^{-\beta\omega_\alpha}} \dot{\chi}_{wv_1}(\tau_2) \\
&= \mathrm{Re}\, \frac{1}{\pi} \sum_{u_1 v_1} \int_{-\infty}^{\infty} \mathrm{d}\omega\, \frac{\tilde{\phi}^{(-)}_{\alpha v_1 u_1}(\omega)}{1 - e^{-\beta\omega_\alpha}} \Big(\int_0^t \mathrm{d}\tau_1\, \dot{\chi}_{vu_1}(\tau_1) e^{-i\omega\tau_1} \Big) \Big(\int_0^t \mathrm{d}\tau_2\, \dot{\chi}_{wv_1}(\tau_2) e^{i\omega\tau_2} \Big) \\
&\to \mathrm{Re}\, \frac{1}{\pi} \sum_{u_1 v_1} \int_{-\infty}^{\infty} \mathrm{d}\omega\, \frac{\tilde{\phi}^{(-)}_{\alpha v_1 u_1}(\omega)}{1 - e^{-\beta\omega_\alpha}} \Big(i\omega \chi^*_{vu_1}(\omega) \Big) \Big(-i\omega \chi_{wv_1}(\omega) \Big),
\end{aligned} \tag{S149}$$

which recovers Eq. (S147b). We also have

$$\gamma_{\alpha uv}(\mathrm{eq}) = \sum_{w} \big[\Omega_{uw}(\infty) k^{10}_{\alpha vw}(\infty) + \Gamma_{uw}(\infty) k^{11}_{\alpha vw}(\infty) \big] + k^{12}_{\alpha uv}(\infty) = \sum_{w} \Gamma_{uw}(\infty) k^{11}_{\alpha vw}(\infty) \tag{S150}$$

which lead to

$$\sum_{\alpha} k^{11}_{\alpha vw}(\infty) = \Gamma_{wv}(\infty) \tag{S151}$$

therefore

$$\sum_{\alpha} \gamma_{\alpha uv}(\mathrm{eq}) = \sum_{w} \Gamma_{uw}(\infty) W^{PP}_{wv}(\mathrm{eq}) \tag{S152}$$

and we obtain

$$\begin{aligned}
\langle \hat{J}^{\mathrm{eq}}_{\alpha} \rangle &= \mathrm{tr}\, \big[\boldsymbol{\Gamma}_{\alpha}(\infty) \boldsymbol{W}^{PP}(\mathrm{eq}) \big] - \mathrm{tr}\, \big[\boldsymbol{\gamma}_{\alpha}(\mathrm{eq}) \big] \\
&= \mathrm{tr}\, \big[\boldsymbol{\Gamma}_{\alpha}(\infty) \sum_{\beta} \boldsymbol{k}^{11}_{\beta}(\mathrm{eq}) \big] - \mathrm{tr}\, \big[\sum_{\beta} \boldsymbol{\Gamma}_{\beta}(t) \boldsymbol{k}^{11}_{\alpha}(\mathrm{eq}) \big]
\end{aligned} \tag{S153}$$

V. NUMERICAL ANALYSIS

Apart from algebraic method, we can also obtain steady state(or equilibrium state) heat current by classical Meir-Wingreen formula

$$J_{\alpha}(\infty) = \frac{2}{\pi} \int_{-\infty}^{\infty} \mathrm{d}\omega\, \frac{\omega}{e^{\beta_\alpha \omega} - 1}\, \mathrm{tr}\, \big[\tilde{\boldsymbol{\phi}}^{(-)}_{\alpha}(\omega) \tilde{\boldsymbol{C}}^{(+)}(\omega) \big] \tag{S154}$$

where $\boldsymbol{C}^{(+)}(\omega)$ is the Hermitian part of the spectrum of correlation functions of the system. In order to obtain correlation function we start from time–nonloacl method, by Eq. 1 and Eq. 2 in the main text we know.

$$\ddot{\hat{Q}}_u(t) = -\sum_{v} V_{uv} \hat{Q}_v(t) + \sum_{\alpha} \hat{F}^{\mathrm{B}}_{\alpha u}(t) + \sum_{\alpha} \int_0^t \mathrm{d}\tau \phi_{\alpha uv}(t - \tau) \hat{Q}_v(\tau), \tag{S155}$$

with $C_{uv} \equiv \mathrm{tr}_{\mathrm{T}}\left[\hat{Q}_u(t)\hat{Q}_v(0)\rho_{\mathrm{T}}^{\mathrm{st}}\right]$ we obtain

$$\begin{aligned}\ddot{C}_{uw}(t) &= -\sum_v V_{uv}C_{vw}(t) + \sum_\alpha \left\langle \hat{F}^{\mathrm{B}}_{\alpha u}(t)\hat{Q}_w(0)\right\rangle + \sum_\alpha \int_0^t \mathrm{d}\,\tau\phi_{\alpha uv}(t-\tau)C_{vw}(\tau)\\ &= -\sum_v V_{uv}C_{vw}(t) + \sum_\alpha X_{\alpha uw}(t) + \sum_\alpha \int_0^t \mathrm{d}\,\tau\phi_{\alpha uv}(t-\tau)C_{vw}(\tau)\end{aligned} \tag{S156}$$

here $X_{\alpha uv}(t) \equiv \left\langle \hat{F}^{\mathrm{B}}_{\alpha u}(t)\hat{Q}_v(0)\right\rangle$ and from entanglement theorem

$$X_{\alpha uv}(t) = -2\sum_w \mathrm{Im}\int_0^\infty d\tau c_{\alpha wu}(t+\tau)C_{vw}(\tau)d\tau \tag{S157}$$

. Equivalently

$$\ddot{\boldsymbol{C}}(t) = -\boldsymbol{V}\boldsymbol{C}(t) + \sum_\alpha \boldsymbol{X}_\alpha(t) + \sum_\alpha \int_0^t \mathrm{d}\,\tau\tilde{\boldsymbol{\phi}}_\alpha(t-\tau)\boldsymbol{C}(\tau) \tag{S158a}$$

$$\boldsymbol{X}_\alpha(t) = -2\,\mathrm{Im}\int_0^\infty \mathrm{d}\tau\, \boldsymbol{c}_\alpha^{\mathrm{T}}(t+\tau)\boldsymbol{C}^{\mathrm{T}}(\tau) \tag{S158b}$$

note that

$$\begin{aligned}\int_0^\infty \mathrm{d}t\,\ddot{\boldsymbol{C}}(t)e^{i\omega t} &= \dot{\boldsymbol{C}}(t)e^{i\omega t}\Big|_0^\infty - i\omega\int_0^\infty \mathrm{d}t\,\dot{\boldsymbol{C}}(t)e^{i\omega t}\\ &= -\dot{\boldsymbol{C}}(0) - i\omega\left[\boldsymbol{C}(t)e^{i\omega t}\Big|_0^\infty - i\omega\int_0^\infty \mathrm{d}t\,\boldsymbol{C}(t)e^{i\omega t}\right]\\ &= -\dot{\boldsymbol{C}}(0) + i\omega\boldsymbol{C}(0) - \omega^2\tilde{\boldsymbol{C}}(\omega)\end{aligned} \tag{S159}$$

therefore Eq. (S156) also leads to

$$\tilde{\boldsymbol{C}}(\omega) = \left[\boldsymbol{V} - \omega^2\mathbf{I} - \sum_\alpha \tilde{\phi}_\alpha(\omega)\right]^{-1}\left[\dot{\boldsymbol{C}}(0) - i\omega\boldsymbol{C}(0) + \sum_\alpha \tilde{\boldsymbol{X}}_\alpha(\omega)\right]. \tag{S160}$$

Eq. (S160) is hard to solve directly so we introduce special method to deal with it. First we expand bath correlation functions $c_{\alpha uv}(t)$ into exponential function.

$$c_{\alpha uv}(t) = \sum_k g_{\alpha uvk}e^{-\gamma_{\alpha k}t} \to \boldsymbol{c}_\alpha(t) = \sum_k \boldsymbol{g}_{\alpha k}e^{-\gamma_{\alpha k}t} \tag{S161}$$

in general $\gamma_{\alpha uvk}$ is independent from u, v so we denote it as $\gamma_{\alpha k}$. In this section, for simplicity we adopt Drude bath,

$$\tilde{\boldsymbol{\phi}}_\alpha(\omega) = \frac{i\gamma_\alpha\boldsymbol{\eta}_\alpha}{\omega + i\gamma_\alpha}, \tag{S162}$$

with this function form of bath, it can be proven that $\{\gamma_{\alpha k}\}$ are always real, therefore many important expressions can be further simplified. Put Eq. (S161) into Eq. (S157) we can recast $\boldsymbol{X}_\alpha(t)$ as

$$\begin{aligned}\boldsymbol{X}_\alpha(t) &= -2\,\mathrm{Im}\int_0^\infty \mathrm{d}\tau\,\boldsymbol{c}_\alpha^{\mathrm{T}}(t+\tau)\boldsymbol{C}^{\mathrm{T}}(\tau)\\ &= -2\,\mathrm{Im}\int_0^\infty \mathrm{d}\tau\,\sum_k \boldsymbol{g}_{\alpha k}^{\mathrm{T}}e^{-\gamma_{\alpha k}(t+\tau)}\boldsymbol{C}^{\mathrm{T}}(\tau)\\ &= -\sum_k e^{-\gamma_{\alpha k}t}\times 2\,\mathrm{Im}\,\boldsymbol{g}_{\alpha k}^{\mathrm{T}}\int_0^\infty \mathrm{d}\tau\, e^{-\gamma_{\alpha k}\tau}\boldsymbol{C}^{\mathrm{T}}(\tau)\\ &= -\sum_k e^{-\gamma_{\alpha k}t}\times 2\,\mathrm{Im}\,\boldsymbol{g}_{\alpha k}^{\mathrm{T}}\tilde{\boldsymbol{C}}^{\mathrm{T}}(i\gamma_{\alpha k})\\ &= -\sum_k e^{-\gamma_{\alpha k}t}\times 2\,\mathrm{Im}\left[\tilde{\boldsymbol{C}}(i\gamma_{\alpha k})\boldsymbol{g}_{\alpha k}\right]^{\mathrm{T}},\end{aligned} \tag{S163}$$

here we formally define

$$\tilde{\boldsymbol{C}}(i\gamma_{\alpha k}) \equiv \int_0^\infty \mathrm{d}\tau\, e^{-\gamma_{\alpha k}\tau}\boldsymbol{C}(\tau) \tag{S164}$$

from Eq. (S163) we get

$$\tilde{\boldsymbol{X}}_\alpha(\omega) = -\int_0^\infty \mathrm{d}t\, e^{i\omega t}\boldsymbol{X}_\alpha(t) = -\sum_k \frac{2}{\gamma_{\alpha k} - i\omega}\,\mathrm{Im}\left[\tilde{\boldsymbol{C}}(i\gamma_{\alpha k})\boldsymbol{g}_{\alpha k}\right]^{\mathrm{T}}. \tag{S165}$$

Let $\omega = i\gamma_{\alpha' k'}$ in Eq. (S165) and along with Eq. (S160) we obtain following equations

$$\tilde{\boldsymbol{X}}_\alpha(i\gamma_{\alpha' k'}) = -\sum_k \frac{2}{\gamma_{\alpha' k'} + \gamma_{\alpha k}}\,\mathrm{Im}\left[\tilde{\boldsymbol{C}}(i\gamma_{\alpha k})\boldsymbol{g}_{\alpha k}\right]^{\mathrm{T}} \tag{S166a}$$

$$\tilde{\boldsymbol{C}}(i\gamma_{\alpha' k'}) = \left[\boldsymbol{V} + \gamma_{\alpha' k'}^2\mathbf{I} - \sum_\alpha \tilde{\phi}_\alpha(i\gamma_{\alpha' k'})\right]^{-1}\left[\dot{\boldsymbol{C}}(0) + \gamma_{\alpha' k'}\boldsymbol{C}(0) + \sum_\alpha \tilde{\boldsymbol{X}}_\alpha(i\gamma_{\alpha' k'})\right], \tag{S166b}$$

from the equations above we can solve $\tilde{C}(i\gamma_{\alpha k})$ for all α and k, on top of which we obtain $\tilde{\boldsymbol{X}}_\alpha(\omega)$. By Eq. (S160) we get the correlation functions for the system. Besides, the initial value of correlation functions can be evaluated from Eq. (S121)

$$\dot{C}_{uv}(0) \equiv \left\langle \hat{P}_u(\infty)\hat{Q}_v(\infty)\right\rangle = W_{uv}^{PQ}(\infty) - \frac{i}{2}\delta_{uv} \tag{S167a}$$

$$C_{uv}(0) \equiv \left\langle \hat{Q}_u(\infty)\hat{Q}_v(\infty)\right\rangle = W_{uv}^{QQ}(\infty), \tag{S167b}$$

here we used condition that $\left\langle \hat{P}_u(\infty)\right\rangle = \left\langle \hat{Q}_u(\infty)\right\rangle = 0$.