A statistical quasi-particles thermofield theory with Gaussian environments: System–bath entanglement theorem for nonequilibrium correlation functions

Yao Wang,* Zi-Hao Chen, Rui-Xue Xu, Xiao Zheng, and YiJing Yan†
Department of Chemical Physics, University of Science and Technology of China, Hefei, Anhui 230026, China
(Dated: August 4, 2022)

For open quantum systems, Gaussian environmental dissipative effect can be represented by statistical quasi-particles, namely dissipatons. We exploit this fact to establish the dissipaton thermofield theory. The resulting generalized Langevin dynamics of absorptive and emissive thermofield operators are effectively noise–resolved. This greatly facilitates establishing the relations between various nonequilibrium Green’s functions or correlation functions, as demonstrated in this work. This is named as system–bath entanglement theorem for nonequilibrium steady–state correlation functions. Here, the phrase of “system–bath entanglement” justifies the context where there exists coherence between system and bath, constituting a type of many–particle composite [30]. All above mentioned relations are validated numerically.

Moreover, the DTF dynamics agrees well with the dissipaton equation of motion (DEOM) theory [31–33], a second–quantization version of the hierarchical equations of motion formalism. It is also noticed that DEOM is practically equivalent to the emerging discrete pseudo-mode semi-group form of the reduced core–system dynamics method [34–37]. Therefore, the proposed DTF theory that integrated with DEOM will serve as a versatile tool for the thermal effects in strongly correlated systems. For brevity, we set throughout this paper $\hbar = 1$ and $\beta_a = 1/(k_B T_a)$, with $T_a$ being the temperature of the $a$th reservoir and $k_B$ the Boltzmann constant.

II. BACKGROUND

Let us start with the total system–plus–reservoirs composite Hamiltonian,

$$H_I = H_S + H_{SB} + H_B, \quad \text{with} \quad H_{SB} = \sum_{\alpha,u} \hat{Q}_\alpha \hat{F}_{\alpha u}. \quad (1)$$

Both the system Hamiltonian $H_S$ and the dissipative system modes $\{ Q_\alpha \}$ are arbitrary, whereas the hybrid reservoir bath modes $\{ F_{\alpha u} \}$ assume to be linear. This together with noninteracting reservoir model of $h_u = \sum_a h_a$ constitute the Gaussian environment ansatz [38, 39]. The environmental influence is fully characterized by the interacting bath reservoir correlation functions ($t \geq 0$):

$$c_\alpha(t) = \{ c_{\alpha uv}(t) = \langle \hat{F}_{\alpha u}(t) \hat{F}_{\alpha v}(0) \rangle_B \}. \quad (2)$$

Here, $\hat{F}^b_{\alpha u}(t) \equiv e^{i h_B t} \hat{F}_{\alpha u} e^{-i h_B t} = e^{i h_B t} \hat{F}_{\alpha u} e^{-i h_B t}$ and $\langle (\cdot) \rangle_B \equiv \text{tr}_B \{ (\cdot) \rho^b_0 \}$ with $\rho^b_0 = \otimes_\alpha [ e^{-\beta_a h_a} / \text{tr}_a ( e^{-\beta_a h_a} ) ]$.
The corresponding response functions are

$$\phi_\alpha(t) = \{\phi_{\alpha uv}(t) \equiv i[\hat{F}^{n}_{\alpha uv}(t), \hat{F}^{n}_{\alpha uv}(0)]_B\},$$

satisfying \(\phi_{\alpha uv}(t) = i[c_{\alpha uv}(t) - c'_{\alpha uv}(t)]\). Inversely, \(c_\alpha(t)\) can also determined by \(\phi_\alpha(t)\) via the fluctuation–dissipation theorem [38–41].

Consider now the \(H_r\)-based Heisenberg picture of the hybrid bath modes. It is easy to obtain [30, 42]

$$\hat{F}_{\alpha uv}(t) = \hat{F}^{n}_{\alpha uv}(t) - \sum_v \int_0^t d\tau \phi_{\alpha uv}(t - \tau) \hat{Q}_v(\tau),$$

with the Langevin random force \(\hat{F}^{n}_{\alpha uv}(t)\) on the local system dissipative mode \(\hat{Q}_u\); see Eq. (1). In other words, Eq. (4) is the precursor to conventional quantum Langevin equation. It together with \([\hat{F}^{n}_{\alpha uv}(t), \hat{Q}_u(0)] = 0\) give rise to the system–bath entanglement theorem for response functions, which is a type of input–output relations in the total composite space [30]. On the other hand, \(\langle \hat{F}^{n}_{\alpha uv}(t)\hat{Q}_v(0) \rangle \neq 0\). To obtain the nonequilibrium steady–state correlation function type input–output relations for such as

$$C_{\alpha \gamma}(t) = \{C^{ss}_{\alpha \gamma}(t) \equiv \langle \hat{Q}_\alpha(t)\hat{Q}_\gamma(0) \rangle\},$$

$$C_{\alpha \gamma}(t) = \{C^{ss}_{\alpha \gamma}(t) \equiv \langle \hat{F}_{\alpha uv}(t)\hat{Q}_v(0) \rangle\},$$

Eq. (4) is insufficient since it cannot distinguish the absorptive and emissive contributions. More specifically, from Eq. (4) we have

$$C_{\alpha \beta}(t) = X_{\alpha \beta}(t) - \int_0^t d\tau \phi_\alpha(t - \tau) \cdot C_{\alpha \beta}(\tau),$$

with

$$X_{\alpha \beta}(t) = \{X^{ss}_{\alpha \beta}(t) \equiv \langle \hat{F}^{n}_{\alpha uv}(t)\hat{Q}_v(0) \rangle\},$$

to be further resolved. To that end, we exploit the statistical quasi-particles picture, which is used in the DEOM theory [31], and obtain

$$X_{\alpha \beta}(t) = \sum_k X_{\alpha \beta k}(t),$$

with

$$X^{ss}_{\alpha \beta k}(t) \equiv \langle \hat{f}^{n}_{\alpha \beta k}(t)\hat{Q}_v(0) \rangle = \langle \hat{f}_{\alpha \beta k}(0)\hat{Q}_v(0) \rangle e^{-\gamma_{\alpha \beta} t}.$$ (9)

Here, \(\{\gamma_{\alpha \beta}\}\) originates from the exponential decomposition of the interacting bath correlations reading [32]

$$c_{\alpha uv}(t) = \sum_k \eta_{\alpha uvk} e^{-\gamma_{\alpha \beta} t}.$$ (10)

Evidently, to establish the aforementioned correlation function type input–output relations, the key step is to formulate \(X^{ss}_{\alpha \beta k}(0)\) in terms of \(C_{ss}(t)\) [cf. Eq. (5a)] and \(c_\alpha(t)\) [cf. Eq. (2)]. We address this issue within the scope of DTF theory to be elaborated as follows.

FIG. 1. An illustrative depiction of the DTF decomposition, exemplified with the case of single reservoir and single coupling mode. Before the decomposition, the hybrid reservoir mode obeys Eq. (4). After the decomposition, statistical quasi–particles evolve as Eq. (14).

III. DISSIPATON THERMOFIELD THEORY

A. Ansatzes

The proposed DTF theory is based on the dissipaton decomposition of the hybrid reservoir modes, as schematically represented in Fig.1. There are three basic ingredients:

(i) Dissipaton decomposition ansatz: The hybrid reservoir modes can be decomposed into dissipators as

$$\hat{F}_{\alpha uv} = \sum_k \hat{f}_{\alpha uv k},$$ (11a)

with [cf. Eqs. (2) and (10)]

$$\langle \hat{f}_{\alpha uv k}(t)\hat{f}^{\dagger}_{\alpha uv k}(0) \rangle_B = \delta_{\alpha \alpha'}\delta_{kk}\gamma_{\alpha uvk} e^{-\gamma_{\alpha uv} t},$$

$$\langle \hat{f}_{\alpha uv k}(0)\hat{f}^{\dagger}_{\alpha uv k}(t) \rangle_B = \delta_{\alpha \alpha'}\delta_{kk}\gamma_{\alpha uvk}^* e^{-\gamma_{\alpha uv} t},$$ (11b)

satisfying \(\langle \hat{f}^{\dagger}_{\alpha uv k}(0)\hat{f}_{\alpha uv k}(0) \rangle_B = \langle \hat{f}_{\alpha uv k}(t)\hat{f}^{\dagger}_{\alpha uv k}(0) \rangle_B^*\), the time–reversal relation, where \(\gamma_{\alpha uvk} \equiv \gamma_{\alpha uvk}\) and \(\hat{f}_{\alpha uv k}(t) \equiv e^{i\hat{H}_{dt} t}\hat{f}_{\alpha uv k} e^{-i\hat{H}_{dt} t}\). This defines dissipators that are statistically independent diffusive environmental modes, exploited previously in the DEOM theory [31].

(ii) Thermofield dissipator ansatz: Each \(\hat{f}_{\alpha uv k}\) consists of an absorptive (+) and an emissive (–) parts,

$$\hat{f}_{\alpha uv k} = \hat{f}^+_\alpha + \hat{f}^-_\alpha,$$ (12a)

defined via

$$\hat{f}^-_{\alpha uv k} \rho_0 = \rho_0 \hat{f}^+_\alpha = 0.$$ (12b)

This results in

$$c^-_{\alpha uvk} = \langle \hat{f}^-_{\alpha uv k}\hat{f}^{-\dagger}_{\alpha uv k}(0) \rangle_B = \eta^-_{\alpha uvk} e^{-\gamma_{\alpha uv} t},$$

$$c^+_{\alpha uvk} = \langle \hat{f}^-_{\alpha uv k}(0)\hat{f}^{\dagger+}_{\alpha uv k}(0) \rangle_B = \eta^+_{\alpha uvk} e^{-\gamma_{\alpha uv} t},$$ (13)

where \(\eta^-_{\alpha uvk} \equiv \eta_{\alpha uvk}\) and \(\eta^+_{\alpha uvk} \equiv \eta^*_{\alpha uvk}\). As the thermofield excitation is concerned [29], \(\hat{f}^-_{\alpha uv k}\) resembles the
creation/annihilation operator onto the reference $\rho_0^\text{init}$ that participates in Eqs. (2) and (11b).

(iii) Thermofield Langevin ansatz: Each thermofield dissipaton satisfies

$$\hat{f}^\pm_{\alpha uk}(t) = \hat{f}^\pm_{\alpha uk}(0) + i \sum_v \int_0^t d\tau c^\pm_{\alpha uvk}(t - \tau) \hat{Q}_v(\tau). \quad (14)$$

In compared with Eq. (4), the resolved are not only the absorptive versus emissive contributions, but also the Langevin force that reads $\hat{f}^\pm_{\alpha uk}(t) = \hat{f}^\pm_{\alpha uk}(0) e^{-\gamma_\alpha k t}$. This recovers the generalized diffusion equation of the DEOM theory [31], further including the thermal effects.

### B. System–bath entanglement theorem for correlation functions

In the following, we elaborate above basic ingredients of the DTF theory, with a class of input–output relations between local and nonlocal nonequilibrium steady–state correlation functions. Denote $C_{\alpha sk}(t) = \{C_{\alpha sk}(t) \equiv \langle \hat{f}_{\alpha uk}(t) \hat{Q}_v(0) \rangle \}$ and $\phi_{\alpha k}(t) = i [c^\pm_{\alpha uk}(t) - c^\pm_{\alpha uk}(t)] = \{\phi_{\alpha uvk}(t) = i [c^-_{\alpha uvk}(t) - c^+_{\alpha uvk}(t)]\}$. Equations (12) and (14) give rise to

$$C_{\alpha sk}(t) = X^\alpha_{uvk}(t) - \int_0^t d\tau \phi_{\alpha k}(t - \tau) \cdot C^\alpha_{ss}(\tau) \quad (15)$$

where $X_{uvk}^\alpha(t) = X_{uvk}^\alpha(0) e^{-\gamma_\alpha k t}$, Eq. (9), and

$$X_{uvk}(0) = i \int_0^\infty d\tau [c^+_{\alpha k}(\tau) C_{ss}^T(\tau) - c^-_{\alpha k}(\tau) C_{ss}^T(\tau)]. \quad (16)$$

with $M^T$ being the matrix transpose. Together with Eq. (15) and (9), we obtain further

$$X^\alpha_{uvk}(t) = 2 \text{Im} \int_0^\infty d\tau c^\alpha_{ov}(t + \tau) \cdot C^T_{ss}(\tau). \quad (17)$$

This completes Eq. (6), the system–bath entanglement theorem for nonequilibrium steady–state correlation functions.

The derivations of the key expression (16) are as follows. (i) Let us start with $\langle \hat{A}(0) \rangle = \lim_{t \to \infty} \text{Tr} [\hat{A}(t) \rho_0^\text{init}]$ for any operator $\hat{A}$. This asymptotic identity holds for any physically supported initial total composite density operator $\rho_0^\text{init}$. In particular, we choose $\rho_0^\text{init} = \rho^\text{init}_0 \otimes \rho^\text{init}_w$, with $\rho^\text{init}_0$ being the pure bath canonical ensemble density operator; (ii) Then split $X_{uvk}^\alpha(0) \equiv \langle \hat{f}_{\alpha uk}(0) \hat{Q}_v(0) \rangle = \langle \hat{f}^+_{\alpha uk}(0) \hat{Q}_v(0) \rangle + \langle \hat{Q}_v(0) \hat{f}^-_{\alpha uk}(0) \rangle$. This is true since the system and reservoir operators are commutable at any given local time; (iii) Finally, obtain $\text{Tr} [\hat{f}^+_{\alpha uk}(t) \hat{Q}_v(t) \rho^\text{init}_0]$ and $\text{Tr} [\hat{Q}_v(t) \hat{f}^-_{\alpha uk}(t) \rho^\text{init}_0]$ from Eq. (14), with focus on their $t \to \infty$ expressions, where $\hat{f}^\pm_{\alpha uk}(t)$ makes no contribution according to Eq. (12b). The resulting $X_{uvk}^\alpha(0)$ according to (ii) is just Eq. (16).

![FIG. 2. Numerical validation of Eq. (15) with Eq. (16) via the equality between lhs (direct) and rhs (indirect) of it, exemplified with two different dissipaton modes, (left and right panel). For simplicity, we adopt $H_S = \hat{\Delta}_0 \hat{\sigma}_s + \frac{1}{2} \hat{\sigma}_x$ and $\hat{Q} = \Delta \hat{\sigma}_x$. The bath spectral density assumes $J(\omega) = (\omega_\text{th}\zeta) / [1/(\omega^2 - \omega_\text{th}^2 + \zeta^2\omega^2)]$, which is related to the interacting bath reservoir correlation functions in Eq. (2) via the fluctuation–dissipation theorem. Parameters are $V = \omega_\text{th} = \zeta = k_B T = \Delta$.](image)

### C. Comments

**a. DTF versus DEOM.** It is worth emphasizing that the present DTF formalism, Eqs. (11)–(14), is rather general in relation to the absorptive and emissive processes. Its application to obtain Eqs. (15)–(17) is an example that can be numerically verified by DEOM evaluations; see Fig. 2 for the direct versus indirect calculations. However, Eqs. (15)–(17) can not be obtained within the original DEOM framework. That is to say, although both the DTF theory and DEOM method are numerically exact for Gaussian environments, DTF theory helps reveal more explicit relations.

Note that the present DTF goes with the exponential decomposition, Eq. (10); see in such as Ref. 43 for the latest developments of exponential decomposition methods. Its generalization to the generic time–derivative closure decomposition scheme [27, 44–49] can be readily constructed, similar to what we have done for the DEOM theory [7]. Nevertheless, the exponential decomposition is often the choice towards the interpretation of experimental observations. Besides, due to the obtained relation (15)–(17), we can compute $C_{\alpha sk}(t)$ by only evaluating $C_{ss}(t)$. The latter is much easier to converge in DEOM calculations. This will help save a lot of numerical costs.

**b. DTF versus NEGF.** Furthermore, the $t = 0$ behaviour of Eq. (6) with Eq. (17) is closely related to the NEGF formalism of transport current [9–11, 17, 18]. For example, consider the heat transport from the alpha–reservoir to the local impurity system. The heat current operator reads

$$\hat{J}_\alpha = \frac{-d\hat{h}_\alpha}{dt} = -i [\hat{H}_T, h_\alpha] = \sum_u F_{au} \hat{Q}_u. \quad (18)$$
This is the electron transport analogue [50, 51]. The heat current is then [cf. Eq. (5b)]

\[ J_\alpha = \sum_u \langle \hat{P}_\alpha u \hat{Q}_u \rangle = \sum_u \hat{C}_{uu}^{\alpha \bar{\alpha}}(t = 0). \]  

(19)

Now apply Eq. (6), with noticing that its second term does not contribute to \( \hat{C}_{uu}^{\alpha \bar{\alpha}}(0) \). We obtain [42]

\[ J_\alpha = 2 \text{Im} \int_0^\infty d\tau \text{tr} \left[ \hat{\xi}_\alpha(\tau) \cdot \hat{C}_{SS}(\tau) \right]. \]  

(20)

This is the time-domain Meir–Wingreen’s formula via the NEGF approaches [9]. It is obtained in NEGF formalism by introducing the contour ordering, followed by the use of Langreth’s rules. Here, the DTF theory can produce it in a rather simple manner. It is worth noting that in the nonequilibrium scenario, the definition of current in Eq. (18) seems to be limited in the weak system–bath coupling [52], but the polaron transformation can take into account of the system–bath interactions non-perturbatively beyond this limitation [53].

c. DTF versus conventional thermofield approach

Last but not least, we compare the DTF theory to the conventional thermofield approach [29]. The thermofield theory has been extended to open quantum dynamics systems, and some studies have been conducted in combination with the hierarchical equations of motion formalism [54–57]. It goes by the purifications of the canonical thermal state, taking the single reservoir and single coupling mode case as an example, as \( |\xi_j\rangle = \prod_j |\xi_j\rangle \), where \( |\xi_j\rangle = (1/\sqrt{Z_j}) \sum_n e^{-\beta_n \omega_j/2} |n_j\rangle \otimes |n_j\rangle' \). With the partition function \( Z_j = (1 - e^{-\beta_j})^{-1} \), the \( |\xi_j\rangle \) is a purification of the density operator \( \rho_j = e^{-\beta_j a_j^{\dagger} a_j} / Z_j = \sum_n (e^{-\beta_n \omega_j} / Z_j) |n_j\rangle \otimes |n_j\rangle' \). Here \( |n_j\rangle' \equiv \frac{1}{\sqrt{\nu_j}} (b_j^{\dagger})^{n_j} |0\rangle' \) and \( |n_j\rangle \equiv \frac{1}{\sqrt{\nu_j}} (b_j^{\dagger})^{n_j} |0\rangle \), with \( a_j^{\dagger} / a_j \) and \( b_j^{\dagger} / b_j \) being the creation/annihilation operators of the original and assistant Fock space, respectively. The vacuum states are defined by \( a_j |0\rangle = b_j |0\rangle = 0 \). It is easy to verify that \( \rho_j = \text{tr} \{ |\xi_j\rangle \langle \xi_j| \} \), where \( \text{tr} \) represents the partial trace with respect to the assistant degrees of freedom. Then, to obtain the zero temperature effective bath, we do the Bogoliubov transformation, which reads

\[ a_j = \sqrt{1 + \bar{n}_j} c_j + \sqrt{\bar{n}_j} d_j, \]  

(21a)

\[ b_j = \sqrt{1 + \bar{n}_j} d_j + \sqrt{\bar{n}_j} c_j, \]  

(21b)

where \( \bar{n}_j = (e^{\beta_j \omega_j} - 1)^{-1} \) is the average occupation number. It can be shown that \( c_j \langle \xi_j| = d_j \langle \xi_j| = 0 \), together with the bosonic commutation relation for \( c_j^{\dagger} \) and \( d_j^{\dagger} \). Now we can add an assistant bath for each reservoir, which does not affect the original system–environment dynamics. It results in \( \hat{h}_n = \sum_j \omega_j (a_j^{\dagger} a_j - b_j^{\dagger} b_j) = \sum_j \omega_j (c_j^{\dagger} c_j - d_j^{\dagger} d_j) \). After Bogoliubov transformation, Eqs. (21a) and (21b), the total Hamiltonian becomes \( \hat{H}_n = \hat{H}_u + \hat{Q} \hat{F} + \hat{h}_n' \), where

\[ \hat{F} = (1/\sqrt{2}) \sum_j g_j (a_j + a_j^{\dagger}) = \hat{F}^+ + \hat{F}^-, \]  

(22)

with

\[ \hat{F}^- |\xi\rangle = (\xi| \hat{F}^+ = 0. \]  

(23)

Here,

\[ \hat{F}^\sigma \equiv (1/\sqrt{2}) \sum_j g_j (\sqrt{1 + \bar{n}_j} c_j^{\dagger} + \sqrt{\bar{n}_j} d_j^{\dagger}) \]  

(24)

satisfies

\[ \hat{F}^\sigma (\tau) = \hat{F}^\sigma(t) - \sigma i \int_0^t d\tau' c^\rho (t - \tau) \hat{Q}(\tau), \]  

(25)

with \( c^\rho(t) = [c(t)]^* = [c^*(t)]^* \) and \( \hat{F}^\sigma(t) = \sum_j (g_j / \sqrt{2}) (\sqrt{1 + \bar{n}_j} c_j^{\dagger} e^{\sigma \omega_j t} + \sqrt{\bar{n}_j} d_j^{\dagger} e^{-\sigma \omega_j t}) \). Comparing between the conventional thermofield and the DTF formalism, we may observe Eqs. (11)–(12) with Eq. (14) as the statistical quasi-particle analogue to Eqs. (22)–(23) with Eq. (25). The present theory would be better physically supported since the introduced discrete statistical quasi-particle picture, with the Langevin force in Eq. (14) being effectively resolved. This agrees with the generalized diffusion equation of the DEOM theory [31].

**IV. CONCLUDING REMARKS**

In conclusion, we develop a statistical quasi-particle thermofield theory, the DTF theory, which is exact assuming the Gaussian influence environments. It goes with the dissipaton decomposition of the hybrid bath reservoir mode. The DTF theory bridges the NEGF and the real–time reduced system dynamics methods. Universal relations for a class of important nonequilibrium steady–state correlation functions are established. The fermionic counterparts to the present DTF theory and the resulting nonequilibrium system–bath entanglement theorem can be readily established in a similar manner. It is also interesting to investigate its deep relationship to the stochastic formalism of quantum dissipation, where the quantum noise appears naturally and the moments of noise lead to a set of generalized hierarchical equations [45, 46]. Generally speaking, the DTF theory is an important ingredient in the study of open quantum systems and will serve as a versatile tool to such as the nonequilibrium thermodynamics and transport phenomena in strongly correlated systems.

**ACKNOWLEDGMENTS**

Support from the Ministry of Science and Technology of China (Grant No. 2017YFA0204904 and
[36] F. Chen, E. Arrigoni, and M. Galperin, “Markovian treatment of non-Markovian dynamics of open Fermionic systems,” New J. Phys. 21, 123035 (2019).

[37] N. Lambert, S. Ahmed, M. Cirio, and F. Nori, “Modelling the ultra-strongly coupled spin-boson model with unphysical modes,” Nature Comm. 10, 3721 (2019).

[38] U. Weiss, *Quantum Dissipative Systems*, World Scientific, Singapore, 2012, 4th ed.

[39] H. Kleinert, *Path Integrals in Quantum Mechanics, Statistics, Polymer Physics, and Financial Markets*, World Scientific, Singapore, 5th edition, 2009.

[40] X. Zheng, R. X. Xu, J. Xu, J. S. Jin, J. Hu, and Y. J. Yan, “Hierarchical equations of motion for quantum dissipation and quantum transport,” Prog. Chem. 24, 1129 (2012).

[41] Y. J. Yan and R. X. Xu, “Quantum mechanics of dissipative systems,” Annu. Rev. Phys. Chem. 56, 187 (2005).

[42] P. L. Du, Z. H. Chen, Y. Su, Y. Wang, R. X. Xu, and Y. J. Yan, “Nonequilibrium system–bath entanglement theorem versus heat transport,” Chem. J. Chin. Univ. 42, 2155 (2021).

[43] Z.-H. Chen, Y. Wang, X. Zheng, R.-X. Xu, and Y. J. Yan, “Universal time-domain Prony fitting decomposition for optimized hierarchical quantum master equations,” J. Chem. Phys. 156, 221102 (2022).

[44] Z. F. Tang, X. L. Ouyang, Z. H. Gong, H. B. Wang, and J. L. Wu, “Extended hierarchy equation of motion for the spin-boson model,” J. Chem. Phys. 143, 224112 (2015).

[45] C.-Y. Hsieh and J. S. Cao, “A unified stochastic formulation of dissipative quantum dynamics. I. Generalized hierarchical equations,” J. Chem. Phys. 148, 014103 (2018).

[46] C.-Y. Hsieh and J. S. Cao, “A unified stochastic formulation of dissipative quantum dynamics. II. Beyond linear response of spin baths,” J. Chem. Phys. 148, 014104 (2018).

[47] L. Cui, H. D. Zhang, X. Zheng, R. X. Xu, and Y. J. Yan, “Highly efficient and accurate sum–over–poles expansion of Fermi and Bose functions at near zero temperatures: Fano spectrum decomposition scheme,” J. Chem. Phys. 151, 024110 (2019).

[48] H. D. Zhang, L. Cui, H. Gong, R. X. Xu, X. Zheng, and Y. J. Yan, “Hierarchical equations of motion method based on Fano spectrum decomposition for low temperature environments,” J. Chem. Phys. 152, 064107 (2020).

[49] T. Ikeda and G. D. Scholes, “Generalization of the hierarchical equations of motion theory for efficient calculations with arbitrary correlation functions,” J. Chem. Phys. 152, 204101 (2020).

[50] D. H. He, J. Thingna, and J. S. Cao, “Interfacial thermal transport with strong system-bath coupling: A phonon delocalization effect,” Phys. Rev. B 97, 195437 (2018).

[51] L. Song and Q. Shi, “Hierarchical equations of motion method applied to nonequilibrium heat transport in model molecular junctions: Transient heat current and high-order moments of the current operator,” Phys. Rev. B 95, 064308 (2017).

[52] J. Ren, P. Hänggi, and B. Li, “Berry-Phase-Induced Heat Pumping and Its Impact on the Fluctuation Theorem,” Phys. Rev. Lett. 104, 170601 (2010).

[53] D. Z. Xu and J. S. Cao, “Non-canonical distribution and non-equilibrium transport beyond weak system-bath coupling regime: A polaron transformation approach,” Front. Phys. 11, 110308 (2016).

[54] T. Arimitsu, “Quantum Langevin equations and quantum stochastic Liouville equations,” Phys. Lett. A 153, 163 (1991).

[55] T. Arimitsu, M. Ban, and T. Saito, “Stochastic Liouville equation approach within non-equilibrium thermo field dynamics,” Phys. A: Stat. Mech. Appl. 177, 329 (1991).

[56] A. Kobryn, T. Hayashi, and T. Arimitsu, “Quantum stochastic differential equations for boson and fermion systems-method of non-equilibrium thermo field dynamics,” Ann. Phys. 308, 395 (2003).

[57] R. Borrelli, “Density matrix dynamics in twin-formulation: An efficient methodology based on tensor-train representation of reduced equations of motion,” J. Chem. Phys. 150, 234102 (2019).