Energy Flux in Hierarchical Equations of Motion and Its Application to a Three-Level Heat Engine

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We derive the formula of energy flux for the hierarchical equations of motion (HEOM) method with the help of stochastic decoupling technique. The resulting expression is a combination of the terms in the first two layers of the hierarchy. The formula is applied to a three-level “heat engine” coupled respectively to three baths, of which two for heat sources and one for work dump. All the three baths are modeled by collections of harmonic oscillators. We illustrate the proper parameterizing to converge the third bath to the “work-dump” limit. As an example, the effect of the engine parameters on working efficiency is studied.

I. INTRODUCTION

Due to the development of technologies there have been observed in many biological systems that microscopic devices provide similar utilities as normal scale engines do. For instance the photosynthetic reaction center of plant and bacteria produces free energy from two heat sources, the sun and the cold ambiance of the earth, that resembles the functionality of a normal scale heat engine. For other microscopic machines not driven by temperature differences it is also important to develop a perspective of thermodynamics. Despite the obvious pragmatic purposes, theory of heat engine shares the common ground of entropy/information with the now active research fields of quantum information transmission and computation. Heat engine doing work is a major connection bridging the pure mathematical concept of information and the concrete reality. Studying full quantum models of heat engines may give another angle of understanding these fundamental concepts.

Microscopic heat engine is different from their normal scale counterparts. The investigation of heat engines laid its ground on the pursuit of work. In normal scale work is unambiguously defined as the product of force and displacement, the two fundamental concepts of Newtonian mechanics, and can be transformed by ideal machinery to varies forms without change in its quantity. In microscopic scale, however, the fluctuation in force and displacement caused by classical randomness and quantum uncertainty is not negligible. Apart from the apparent analogy to the macroscopic definition of work, it is still unclear how to identify the random output of microscopic heat engines with the deterministic utilities that people demand. More substantially, the interaction of microscopic heat engines with their environments could be stronger than their counterparts. Unlike the classical the-
ory in which engine is well separated from environment and interact weakly to the almost unperturbed heat baths, the microscopic heat engine is virtually embedded into the heat baths. The interaction heavily disturbs both the engine and the heat baths that per se breaks the assumed settings of the classical theory. Therefore it is necessary to bring in more fundamental models and dynamic viewpoints into the study of such scenarios.

There have been various microscopic models of heat engines. Some models like Szilard’s engine [1] and Feynman’s ratchet and pawl [2] are heuristic in giving explicit information mechanisms. Close examinations of them convince people the integration of information processes (e.g. measurement) into thermodynamics is necessary [3]. Also inferred is that information is as well restricted by the laws of thermodynamics [4]. Despite the conceptual importance, their dynamics is not easy to simulate. Some efforts to formalize these models have been made recently [5–9]. In contrast to these heuristic models, there are also engines much easier to simulate. A pioneering one is a model of maser proposed by Scovil and Schulz-Dubios [10] where a simple three-level system is coupled to two heat baths and one work dump. The model is found equivalent to a heat engine and subject to the same Carnot efficiency. This discovery has ignited many following researches [11–13]. Simple as they are, the informational mechanisms of these models are not obvious. We leave such theoretic inquiries to theorists and in the present work limit ourselves to the construction of a reliable numerical method that calculates work and heat flows for such models.

A standard method dealing with such models is the master equation pioneered by Lindblad [14] and Gorini-Kossakowski-Sudarshan [15], and then applied to quantum heat engines by Kosloff [16]. The method consistently reproduces the laws of equilibrium thermodynamics [17] which qualifies it as an eligible generalization of thermodynamics to quantum regime. Despite the quantum nature of the method, its dependence on idealizations like Markovian approximation and weak coupling leaves spaces for improvements. Microscopic heat engine may be tightly embedded into its environments and the time scale separation between the engine and the environment may be invalid. For them the weak coupling assumption and Markovian approximation is over-demanding. Hierarchical equations of motion (HEOM) is a powerful tool to go beyond those approximations. HEOM has been popularized in the last decade [18–21] and has become a benchmark in quantum open system simulations. It is frequently used as a reliable tool to simulate models of finite-state quantum systems coupled to heat baths comprised of harmonic oscillators. HEOM is numerically exact and remarkably
efficient. It does not rely on Markovian approximation, weak coupling, etc. Though its bath model is limited by the requirement of harmonicity, its validity has been argued [22] and tested in many researches. One way of deriving HEOM is through stochastic decoupling [19], which is also the route the present research takes. Stochastic decoupling provides rigorous mathematics to separate two subsystems connected by the interaction of factorized form. The separation provides a convenient framework to calculate the local observables of the interested subsystems. With the help of the above-mentioned tools we find the expression of energy flux in HEOM formalism and then apply it to a three-level heat engine.

The rest of the paper is arranged as follows. Section II derives the expression of energy flux for the system-plus-bath models in the framework of HEOM. Section III applies the general formalism to a three-level heat engine coupled to three baths. The proper parameterizing to converge one of the bath to a work dump is illustrated. Section IV exemplifies the method by calculating the efficiency of the heat engine.

II. THE EXPRESSION OF ENERGY FLUX IN HEOM

Consider a system-plus-bath complex \( H = H_s + H_b + f_s g_b \), where \( H_s \) and \( H_b \) stand for the system Hamiltonian and the bath Hamiltonian respectively. The interaction between the system and the bath is a simple product of a system operator \( f_s \) and a bath operator \( g_b \). The basis of defining a flux is that a flux into the system increases its respective physical quantity. Calling the quantity \( A_s \), we define its flux \( \langle j \rangle = \frac{d}{dt} \langle A_s \rangle \). Using the propagator of the Hamiltonian, it is straightforward to show that \( \langle j \rangle = Tr \{ i [H_s, A_s] \rho (t) \} + Tr \{ ig_b [f_s, A_s] \rho (t) \} \), where the flux operator is identified as \( j = i [H_s, A_s] + ig_b [f_s, A_s] \). The factorization of system operator and bath operator in the expression naturally sees the application of stochastic decoupling technique [23]. To perform that, first we note the total density matrix can be cast in the form \( \rho (t) = M_{u_1, u_2} \{ \rho_s (u_1, u_2^* \rho_b (u_1^*, u_2) \} \), where \( u_{1,2} \) are two white noises. \( \rho_s \) and \( \rho_b \) are operators of, respectively, system space and bath space, both driven by the noises \( u_{1,2} \). With the expression the flux is written as

\[
\langle j \rangle = i Tr_s \{ [H_s, A_s] \hat{\rho}_{s,0} \} + i Tr_s \{ [f_s, A_s] \hat{\rho}_{s,1} \},
\] (1)
where the bath plays its role via

\[ \tilde{\rho}_{s,1} = M_{u_1,u_2} \{ \rho_s T_{rb} \{ \rho_b \} \tilde{g} (t) \} \]
\[ \tilde{\rho}_{s,0} = M_{u_1,u_2} \{ \rho_s T_{rb} \{ \rho_b \} \} . \]  

Notice \( \tilde{\rho}_{s,0} \) is actually the reduced density matrix \( \tilde{\rho}_s \) of the system and \( \tilde{\rho}_{s,1} \) is some correlation between the system and the random force exerted by the bath. \( \rho_s \) is determined by the stochastic differential equation (SDE) \( id\rho_s (t) = [H_s, \rho_s (t)] \, dt + \frac{1}{2} [f_s, \rho_s (t)] \, u_{1,t} \, dt + \frac{i}{2} \{ f_s, \rho_s (t) \} \, u_{2,t} \, dt \), for the bath of Caldeira-Leggett model [22]. The bath part is solved analytically in the form \( \tilde{\rho}_{b,1} \) is solved analytically in the form \( T_{rb} (\rho_b) \) = \[ \int_0^t \alpha_1 (t-\tau) u_{2,\tau} \, dt + \int_0^t \alpha_R (t-\tau) u_{1,\tau}^* \, dt \], and \( \alpha_1, \alpha_R (t) \) is imaginary(real) part of response function \( \alpha (t) = \frac{1}{\pi} \int_0^\infty d \omega \, J (\omega) \, [ \coth (\beta \hbar \omega / 2) \cos (\omega t) - i \sin (\omega t) ] \). \( J (\omega) \) is the spectral density function of the bath. Because the expression is linear in the noise \( u_1 \), \( T_{rb} \{ \rho_b \} \) is absorbed into the weight function of the noise in Eq. [2] with Girsnov transform, which simplifies the expressions to:

\[ \tilde{\rho}_{s,1} = M_{u_1,u_2} \{ \tilde{\rho}_s (t) \tilde{g} (t) \} \]
\[ \tilde{\rho}_{s,0} = M_{u_1,u_2} \{ \tilde{\rho}_s \} . \]

The transform also affects \( \rho_s \) and results in a new density matrix \( \tilde{\rho}_s \) driven by the new SDE

\[ id\tilde{\rho}_s = [H_s, \tilde{\rho}_s] \, dt + [f_s, \tilde{\rho}_s] \tilde{g} (t) \, dt + \frac{1}{2} [f_s, \tilde{\rho}_s] u_{1,t} \, dt + \frac{i}{2} \{ f_s, \tilde{\rho}_s \} u_{2,t} \, dt . \]  

Averaging the equation gives formally \( i \frac{d}{dt} \tilde{\rho}_{s,0} = [H_s, \tilde{\rho}_{s,0}] + [f_s, \tilde{\rho}_{s,1}] \), which straightforwardly validates Eq. [1]. The key quantities \( \tilde{\rho}_{s,0} \) and \( \tilde{\rho}_{s,1} \) could in principle be calculated by propagating and averaging the SDE (Eq.[4]) mentioned above. However, in practice it is indeed obtained via the more efficient HEOM through the connection between the SDE and HEOM that will be detailed later.

For energy flux \( A_s = H_s \), Eq. [1] is reduced to

\[ \langle j \rangle = i Tr_s \{ [f_s, H_s] \tilde{\rho}_{s,1} \} . \]

A slight different way to define energy flux is \( \langle j \rangle = - \frac{d}{dt} \langle H_b \rangle \). The two ways are nonequivalent as, by energy conservation \( - \frac{d}{dt} \langle H_b \rangle = \langle j \rangle + \frac{d}{dt} \langle f_s g_b \rangle \), there is a difference \( \frac{d}{dt} \langle f_s g_b \rangle \). The latter definition, however, is also computable in this framework, only more complicated. To get \( \frac{d}{dt} \langle f_s g_b \rangle \) we start from \( \langle f_s g_b \rangle = Tr \{ \rho f_s g_b \} \) and \( \rho (t) = M_{u_1,u_2} \{ \rho_s (u_1, u_2^*) \rho_b (u_1^*, u_2) \} . \)
Combining the equations above we have \( \langle f_s g_b \rangle = \text{Tr} \left\{ f_s M_{u_1,u_2} \left\{ \rho_s \text{Tr} (\rho_b) \bar{g} (t) \right\} \right\} \), \( \text{Tr} (\rho_b) \) is as usual absorbed with the help of Girsanov transform to get \( \langle f_s g_b \rangle = \text{Tr} \left\{ f_s \bar{\rho}_{s,1} \right\} \). Adding the two parts reveals the expression for the second definition of energy flux to be

\[
\langle j \rangle = -\text{Tr} \left\{ i [H_s, f_s] \bar{\rho}_{s,1} \right\} + \text{Tr} \left\{ f_s \frac{d}{dt} \bar{\rho}_{s,1} \right\}.
\]  

(6)

From the SDE (Eq. (4)), HEOM is derived by working out the ordinary differential equations (ODEs) of the average \( M \left\{ \bar{\rho}_s \right\} \) with help of Ito Calculus [19]. As has been intensively studied and applied to many systems [24–26], HEOM is effective and precise to simulate quantum dissipation systems with fast decaying response functions. Simply saying, the technique splits the response function \( \alpha_{I,R} (t) \) into the sum of exponential functions. Respectively \( \bar{g} (t) \) is also divided into the sum of \( \bar{g}_j (t) \)s, each of which is for one exponential. The collection of averages \( M_{u_1,u_2} \left\{ \bar{\rho}_s \Pi_j \bar{g}_j (t)^{n_j} \right\} \), labeled by indexes \( (n_1, n_2, \cdots) \) \( (n_j \) is a non-negative integer), is determined by a hierarchically related set of ODEs. \( M_{u_1,u_2} \left\{ \bar{\rho}_s \right\} \) (the reduced density matrix) is the leading term with \( (n_1, n_2, \cdots) = (0,0,\cdots) \). The hierarchy is truncated to finite layers \( \sum_j n_j < N \). The cross relations of the coupled ODEs are sparse because any term labeled by \( (n_1, n_2, \cdots) \) is related only to its immediate superior and subordinate terms \( (n_1, n_2, \cdots, n_j \pm 1, n_{j+1}, \cdots) \). This feature contributes to its high numerical efficiency. In most applications of HEOM only the leading term \( \bar{\rho}_{s,0} = M_{u_1,u_2} \left\{ \bar{\rho}_s \right\} \) is required to calculate the system-related quantities as it is the reduced density matrix \( \bar{\rho}_s \) of the system. But for fluxes, \( \bar{\rho}_{s,1} \) (Eq. (5)) and probably \( \frac{d}{dt} \bar{\rho}_{s,1} \) (Eq. (6)) are also needed. It is seen from Eq. (3) that \( \bar{\rho}_{s,1} = \sum_j M_{u_1,u_2} \left\{ \bar{\rho}_s (t) \bar{g}_j (t) \right\} \) is the sum of the second layer terms (with \( \sum_j n_j = 1 \) ) of HEOM. Its derivative \( \frac{d}{dt} \bar{\rho}_{s,1} \) is also known to be a certain combination of the first layer (\( \sum_j n_j = 0 \)) and the third layer (\( \sum_j n_j = 2 \)) terms based on the hierarchical dependence of ODEs. The exact form of \( \frac{d}{dt} \bar{\rho}_{s,1} \) relies on the shapes and the specific splitting of \( \alpha_{I,R} (t) \), thus is not listed generally here. For convenience, we choose the first definition Eq. (1) in thereafter simulations because of its independent form and lesser requirements. The dependence of transportation properties of fermion system on the second layer terms of HEOM is also found in Ref. [27].
III. THEORY FOR A THREE-LEVEL HEAT ENGINE

The three-level heat engine we study is illustrated in Figure 1. A quantum system with three states (labeled by their energy $E_j$) is coupled to three baths (labeled by their temperature $T_{ij}$). Each bath causes the transition between two of the states ($E_i$ and $E_j$) and produces an energy flux $J_{ij}$ in or out of the bath. We choose the incoming flux to the system to be positive and the other direction negative. The baths are Caldeira-Leggett models with friction coefficients $\eta_{ij}$. This model allows for a full quantum description with time-independent Hamiltonian and thus provides some rigors for discussing subtle quantum effects.

A. HEOM for a three-level system

To model the heat engine named above, we need to couple three baths to the engine to transit between its three levels, the Hamiltonian reads:

$$H = H_s + \sum_{ij \in \{12, 23, 13\}} \left( H^{ij}_{b} + f^{ij}_{s} g^{ij}_{b} \right).$$  (7)
The system part is simple diagonal $H_s = \sum_{k=1}^{3} E_k |k><k|$ with energy levels $E_k$. Each bath is a collection of harmonic oscillators $H_b^{ij} = \sum_{\alpha} \left[ \frac{1}{2} m_{ij}^{\alpha} (\omega_{ij}^{\alpha} x_{ij}^{\alpha})^2 + \frac{(p_{ij}^{\alpha})^2}{2 m_{ij}^{\alpha}} \right]$ where $\alpha$ counts the oscillators of a bath and $ij$ refers to the two system levels exchanged by the said bath. The interaction rises between the collective coordinate of the bath oscillators $g_{b}^{ij} = \sum_{\alpha} c_{ij}^{\alpha} x_{ij}^{\alpha}$ and the transition of the system $f_{s}^{ij} = |i><j| + c.c.$ Ito formula helps to verify $\rho(t) = M \left\{ \rho_s \prod_{ij\in\{12,23,13\}} \rho_b^{ij} \right\}$ as the solution of the Liouville equation $i\partial_t \rho = [H, \rho]$. The SDEs for the system and the baths are respectively

$$id\rho_s(t) = [H_s, \rho_s(t)] dt + \frac{1}{2} \sum_{ij} \left[ f_{s}^{ij}, \rho_s(t) \right] u_{1,t}^{ij} dt + \frac{i}{2} \sum_{ij} \left\{ f_{s}^{ij}, \rho_s(t) \right\} u_{2,t}^{ij} dt$$

$$id\rho_b^{ij}(t) = [H_b^{ij}, \rho_b^{ij}(t)] dt + \frac{1}{2} \left[ g_{b}^{ij}, \rho_b^{ij}(t) \right] u_{2,t}^{ij} dt + \frac{i}{2} \left\{ g_{b}^{ij}, \rho_b^{ij}(t) \right\} u_{1,t}^{ij} dt.$$  

The operator $M \{ \cdot \}$ averages its operand over all noises introduced by stochastic decoupling.

Similar to Eq. (1), the fluxes are defined by the change of the system energy $\frac{d}{dt} (H_s) = -i \sum_{ij} \langle g_{b}^{ij} [H_s, f_{s}^{ij}] \rangle = \sum_{r=1}^{3} \langle f_{s}^{ij} \rangle$, here $ij$ notifies the flux being generated by the transition between $|i >$ and $|j >$ states. With $\tilde{\rho}_{s,1}^{ij} = M \left\{ \rho_s g_{b}^{ij} (t) \prod_{r} Tr^{ij} \{ \rho_b^{ij} \} \right\}$ and the same techniques utilized in the previous derivation, the value of the flux $\langle f_{s}^{ij} \rangle = -i Tr \left\{ \rho g_{b}^{ij} [H_s, f_{s}^{ij}] \right\}$ is simplified to an expression in the finite-dimensional reduced space

$$\langle f_{s}^{ij} \rangle = -i Tr \left\{ [H_s, f_{s}^{ij}] \tilde{\rho}_{s,1}^{ij} \right\}, \quad (8)$$

here $\tilde{g}_{b}^{ij}(t) = \int_{t}^{0} [f_{s}^{ij}, \rho_s(t-\tau)] u_{1,t}^{ij} d\tau$, $\int_{0}^{t} [f_{s}^{ij}, \rho_s(t-\tau)] u_{2,t}^{ij} d\tau$. After Girsanov transform absorbs the trace of the bath density matrices, $\tilde{\rho}_{s} = M \{ \tilde{\rho}_{s} \}$ and $\tilde{\rho}_{s,1} = M \{ \tilde{\rho}_{s}(t) \tilde{g}_{b}^{ij}(t) \}$ are calculated from $\tilde{\rho}_{s}$, which is in turn determined by $id\tilde{\rho}_{s} = [H_s, \tilde{\rho}_s] dt + \sum_{ij} \left\{ f_{s}^{ij}, \tilde{\rho}_s \right\} \tilde{g}_{b}^{ij}(t) dt + \sum_{ij} \left\{ \frac{1}{2} [f_{s}^{ij}, \tilde{\rho}_s] u_{1,t}^{ij} dt + \frac{i}{2} \left\{ f_{s}^{ij}, \tilde{\rho}_s \right\} u_{2,t}^{ij} dt \right\}$. Averaging the above SDE, we have $id\tilde{\rho}_{s} = [H_s, \tilde{\rho}_s] dt + \sum_{ij} \left\{ f_{s}^{ij}, \tilde{\rho}_{s,1}^{ij} \right\} dt$, which easily verifies

$$\frac{d}{dt} Tr_s (\tilde{\rho}_s H_s) = \sum_{r} \langle \rho_r^* \rangle. \quad (9)$$

The same manipulation briefed in the previous section transforms the SDEs to HEOM. We utilize HYSHE package to solve the coupled differential equations of HEOM. HYSHE is designed with optimized data structure to solve quantum dynamics of small systems coupled to multiple Caldeira-Leggett baths and time-dependent driven forces. Many truncation policies are implemented in the code to accelerate convergence. We adopt Debye-cutoff $\Omega$-form spectral density function $J(\omega) = \eta \omega \frac{1}{1 + (\omega / \omega_c)^2}$ readily provided in the package for
all three baths. As the original code only records the first layer of the hierarchy (i.e. the reduced density matrix), some lines are amended to capture and process the second layer terms for the deduction of energy fluxes. The modification is, generally saying, minimal.

Though in practice the HYSHE package itself takes the majority of the job, we would like to bring forward the equations playing behind the code to add some transparency to the black box (see also Ref. [24]). For the chosen spectral density the response function is split as:

\[
\alpha(t) = \frac{n \omega_c^2}{2} [\cot(\beta \hbar \omega_c/2) - i] \exp(-\omega_c t) \\
+ \frac{2n \omega_c^2}{\hbar \beta} \sum_{k=1}^{\infty} \frac{v_k \exp(-v_k t)}{v_k^2 - \omega_c^2}
\]

here \(v_k = 2\pi k/(\hbar \beta)\). We denote for clarity the coefficients \(C_0 = \frac{n \omega_c^2}{2} \cot(\beta \hbar \omega_c/2), D_0 = -\frac{n \omega_c^2}{2}\) and \(\omega_0 = \omega_c, C_J = \frac{2n \omega_c^2}{\hbar \beta} \frac{v_J}{v_J^2 - \omega_c^2}\) and \(\omega_J = v_J\) for \(J > 0\), thus the response function is split as \(\alpha(t) = iD_0 \exp(-\omega_0 t) + \sum_{J=0}^{N} C_J \exp(-\omega_J t)\). Respectively \(g(t)\) is expressed as

\[
g(t) = \int_0^t \alpha_I(t - \tau) u_{2,\tau} d\tau + \int_0^t \alpha_R(t - \tau) u_{1,\tau}^* d\tau \\
= \int_0^t D_0 \exp(-\omega_0 (t - \tau)) u_{2,\tau} d\tau + \sum_{J=0}^{N} \int_0^t C_J \exp(-\omega_J (t - \tau)) u_{1,\tau}^* d\tau
\]

where \(g_J(t) = \delta_{J,0} \int_0^t D_0 \exp(-\omega_0 (t - \tau)) u_{2,\tau} d\tau + \int_0^t C_J \exp(-\omega_J (t - \tau)) u_{1,\tau}^* d\tau\). Its derivative is \(d_\tau g_J(t) = \delta_{J,0} D_0 u_{2,\tau} + C_J u_{1,\tau}^* - (\delta_{J,0} \omega_0 \bar{g}_{0,im}(t) + \omega_J \bar{g}_{J,im}(t)) d\tau\) where \(\bar{g}_{0,im}(t) = \int_0^t D_0 \exp(-\omega_0 (t - \tau)) u_{2,\tau} d\tau\), and \(\bar{g}_{J,im}(t) = \int_0^t C_J \exp(-\omega_J (t - \tau)) u_{1,\tau}^* d\tau\). By Ito calculus \((d_\tau g_J(t)) (d_\tau g_K(t)) = 0\) is validated.

To avoid confusion the bath name \(ij \in \{23, 13, 12\}\) will be replaced by \(r \in \{1, 2, 3\}\) here. In this notation we define \(M \left\{ \bar{\rho}_s, \prod_{r=1}^{3} \prod_{J=0}^{N} (\bar{g}_J)_{I,J} \right\} = \bar{\rho}_I\), where the subscript \(I\) itself is a matrix of non-negative integral entries. Utilizing Ito formula and averaging over all auxiliary noises we get

\[
i \frac{d}{dt} \bar{\rho}_I = -i \sum_{m=1}^{3} \sum_{n=0}^{N} I_{m,n} \omega_n^m \bar{\rho}_I + [H_s, \bar{\rho}_I] + \sum_{m=1}^{3} \sum_{n=0}^{N} \left[ f_{s}^{m} \cdot \bar{\rho}_I + \Delta_{m,n} \bar{\rho}_I \right] \\
+ i \sum_{m=1}^{3} I_{m,0} D_0^m \left\{ f_{s}^{m} \cdot \bar{\rho}_I - \Delta_{m,0} \right\} dt + \sum_{m=1}^{3} \sum_{n=0}^{N} I_{m,n} C_{m}^{n} \left[ f_{s}^{m} \cdot \bar{\rho}_I - \Delta_{m,n} \right].
\]
Here $\Delta_{m,n}$ is a matrix defined by its entries $(\Delta_{m,n})_{r,J} = \delta_{mr}\delta_{nJ}$. To calculate the energy flux from bath $r$, any term $\rho_I$ with all $I$'s entries zero, except one single 1 at its $r$'th row, will be summed up to
\[
\tilde{\rho}_{r,1} = \sum_n \tilde{\rho}_{\Delta_{r,n}}.
\] (13)
This expression, along with Eq. (8), calculates the energy flux from the $r$'th bath.

In HYSHE proper factors are multiplied to scale the hierarchical terms for better numerical performance:
\[
P_I = \frac{\prod_r \prod_{J=0}^N (\omega_J^{r})^{I_r,J}}{\left(\prod_r \prod_{J=0}^N (I_r,J!) |C_J^r + i\delta_{J0}D_J^r| I_{r,J}^{r}\right)^{1/2}} \tilde{\rho}_I.
\] (14)
The scaling also changes the hierarchical equations to
\[
id{dt}P_I = -i \sum_{m=1}^3 \sum_{n=0}^N I_{m,n} \omega_n^m P_I + [H_s, P_I]
\] (15)
\[
+ \sum_{m=1}^3 \sum_{n=0}^N (\omega_n^m)^{-1} (I_{m,n} + 1)^{1/2} |C_n^m + i\delta_{n0}D_n^m|^{1/2} \left[f_s^m, P_I + \Delta_{n,m}\right]
\]
\[
+ \sum_{m=1}^3 \sum_{n=1}^N \omega_n^m (I_{m,n})^{3/2} |C_n^m|^{-1/2} C_m^m \left[f_s^m, P_I - \Delta_{n,m}\right]
\]
\[
+ \omega_0^m |C_n^m + iD_0^m|^{-1/2} I_{n,0}^m \sum_{m=1}^3 \left\{iD_0^m \left[f_m^m, P_I - \Delta_{m,0}\right] + C_0^m \left[f_m^m, P_I - \Delta_{m,0}\right]\right\}.
\]
Thus to compensate, its raw output of the second layer terms ought to be scaled back to
\[
\tilde{\rho}_I = P_I \left(\frac{|C_J^r + i\delta_{J0}D_J^r|}{\omega_J^{r}}\right)^{1/2}
\] before Eq. (13) is employed.

B. The parameters of the work-dump

The immediate outputs of HYSHE are time-dependent bath-specific energy fluxes. Their typical look is like Figure 2. We choose the solely occupied ground state of the system to start the propagation. The baths are initially in their factorized equilibrium as required by HEOM. The result of a simulation generally displays plateau of fluxes quickly reached after a short disturbance caused by initial thermalization. Once the steady state builds up, the three fluxes cancel out as implied by Eq. (9). The simulation for Figure 2 takes less than an hour to complete on a single core of Xeon E5 CPU.

Unlike typical engines working in cycles, the three-level “engine” works in a steady state. To catch the steady state, the propagation time is chosen sufficiently long to ensure the effect
Figure 2: The fluxes $J$ versus the time $t$, the parameters set for the simulation are $E_1 = 0$, $E_2 = 0.1$, $E_3 = 0.92$, $T_{12} = 40$, $T_{23} = 3$, $T_{13} = 4$, $\eta_{12} = 0.025$, $\eta_{13} = \eta_{23} = 0.02$ and $\omega_c = 2$ for all three baths.

of the initial state fades away. The final (steady) values of the fluxes are then recorded and studied on their relations to the engine parameters.

Now that we have three steady fluxes, the next task is to assign different roles to them by setting up proper parameters to their baths. For a heat engine two heat sources with relatively higher and lower temperatures are mandatory. The fluxes directed to them balance the entropy ($\frac{\delta E_1}{T_{11}} + \frac{\delta E_2}{T_{22}} = 0$) but leave an energy gap ($\delta E_1 + \delta E_2 \neq 0$). The gap should be offset by another work-dump bath which takes in proper amount of energy ($\delta E_3 = - (\delta E_1 + \delta E_2)$) but no entropy. A mechanic way of setting up such a work-dump is to push against a payload. This generally means to introduce a time-dependent HEOM and some interpretations which we will address in the follow-up works. In this work, we choose the thermodynamic way similar to Ref. [13] to set up the work dump. Simply saying, any energy flowing out of the third bath is accompanied by entropy $\delta S = \frac{\delta E}{T}$. Here $T$ is the temperature of the bath, which also implies the assumption of thermal equilibrium and infinite heat capacity of the bath. It is immediately noticed that setting $T$ to infinity would meet the "energy but no entropy" criteria. In practice the infinitely high temperature can be approximated by a finite but large enough value relative to those of the other two baths. However, as is shown in Figure 3, increasing temperature is not enough by only itself. It depresses the fluxes without a foreseeable non-zero limit while our work-dump bath is expected to have
a fixed non-zero limit of flux. The reason is, we hint, that increasing the temperature not
only projects the bath to its limiting work-dump behavior, but also moves the targeted
limit. To see closer, we first refer to the fact that the effect of the harmonic bath upon
our system is completely depicted by the $\Omega$-form spectral density function $J(\omega)$ and in
turn its response function $\alpha(t) = \frac{1}{\pi} \int_0^\infty d\omega \, \eta \omega C(\omega) \left[ \coth \left( \frac{\beta \hbar \omega}{2} \right) \cos(\omega t) - i \sin(\omega t) \right]$. Here
the cutoff function $C(\omega)$ truncates $J(\omega) = \eta \omega C(\omega)$ to finite bandwidth $\omega_c$. The limiting
work-dump behavior of the bath requires a finite form of $\alpha(t)$ when temperature $T$ goes
to infinity. But exclusively increasing temperature makes an unphysical infinity in the real
part of $\alpha(t)$. To resolve the singularity we observe that the real part of $\alpha(t)$ depends on
$T$ through $\coth \left( \beta \hbar \omega / 2 \right)$ which converges to $2 k_B T / \hbar \omega$ when $T$ is large enough. This feature
prompts that setting the rest engine parameter $\eta$ proportional to $1/T$ makes the anticipated
limit. Without losing generality, we set $\eta = 1/T$ and choose units so that $\hbar, k_B = 1$. For
$T \gg \omega_c$, the real part of $\alpha(t)$ is reduced to a finite $\alpha_R(t) = \frac{2}{\pi} \int_0^\infty d\omega \, C(\omega) \cos(\omega t)$. This, along with $\lim_{T \to \infty} \alpha_I(t) = 0$, defines the limiting work-dump behavior of the bath. The
finite limit of $\alpha(t)$ promises a non-zero intake of energy and $T \to \infty$ ensures no entropy is
attached to the energy. This makes the nature of a work dump. We are aware that the work
dump has a characteristic time scale $\omega_c^{-1}$. Though there is still not a ubiquitous definition
of work consistent throughout all scenarios, it is not surprising that the expected one should
be specific upon its time scale. For example, femtosecond time resolution allows one to track
the forces and displacements of molecules and estimate the work as their products, while
time scale of a second blurs out all details and leaves only heat flux to be observed. To name
the same movement work or heat one must specify its time scale a priori.

In simulation we take the third bath as the work dump, increase its temperature $T_{12}$ and
set $\eta_{12} = 1/T_{12}$ accordingly while keeping the parameters of the other two baths invariant.
The result is displayed in Figure 4. The plateau formed after $T_{12} > 30$ suggests the work-
dump limit be reached when $T_{12}$ is ten times larger than $T_{13}$ and $T_{23}$. In the following
simulations we choose $T_{12}$ large enough to safely converge the third bath and study the
effect of other parameters.
Figure 3: The fluxes $J$ versus the temperature of the work dump $T_{12}$, the parameters set for the simulation are $E_1 = 0$, $E_2 = 0.1$, $E_3 = 0.92$, $T_{23} = 3$, $T_{13} = 4$, $\eta_{12} = 0.025$, $\eta_{13} = \eta_{23} = 0.02$ and $\omega_c = 2$ for all three baths. $T_{12}$ is increased from 4 to 50.

Figure 4: The fluxes $J$ versus the temperature of the work dump $T_{12}$, the parameters set for the simulation are $E_1 = 0$, $E_2 = 0.1$, $E_3 = 0.92$, $T_{23} = 3$, $T_{13} = 4$, $\eta_{13} = \eta_{23} = 0.02$ and $\omega_c = 2$ for all three baths. $T_{12}$ is increased from 4 to 50 and $\eta_{12} = 1/T_{12}$. 
IV. THE EFFICIENCY OF A THREE-LEVEL HEAT ENGINE

As an application of the technique proposed above, we study the effect of the parameters on the efficiency of the engine. To isolate the effect, the parameters related to the work dump need to be fixed first, including $T_{12} = 40$, $T_{23} = 3$, $T_{13} = 4$, $\eta_{12} = 0.025$, $\eta_{13} = \eta_{23} = 0.02$ and $\omega_c = 2$ for all three baths. $E_3$ is increased from 0.2 to 1.04.

The steady flux $J_{12}$, $J_{23}$ and $J_{13}$ are taken from the levels of the plateaus and then fed into the definition $\eta_{\text{eff}} = \frac{-J_{12}}{\text{Max}(J_{13},J_{23})}$ (see Ref. [13]) for the efficiency of the heat engine. For the small coupling strength we choose, the shifts of the energy gaps are negligible, thus the energy flux could be approximated by $I (E_i - E_j)$ where $I$ is the population circulation. The efficiency $\eta_{\text{eff}} = \frac{I(E_2 - E_1)}{\text{Max}(I(E_3 - E_1),I(E_2 - E_3))}$ is then found to be independent of the magnitude of $I$. The sign of $I$ is inferred from the sign of the energy flux $J_{ij}$. This theory is compared to the numerical simulation in Figure 5 and the results fit well to each other. Note that the gap in the efficiency $\eta_{\text{eff}}$ is caused by the switch from refrigerator to heat engine.
V. CONCLUSION

In the framework of stochastic decoupling and for the bath model comprised of harmonic oscillators, we find the expression of energy flux to be determined by the correlation between the random density matrix of the system and the random force exerted by the bath (Eq. (3) and (5)). Through the connection between stochastic decoupling and HEOM we further express the energy flux as a combination of the terms in the second layer of HEOM. The result makes an efficient and numerically exact approach that calculates energy fluxes without approximations. We argue that to converge the bath to a work dump one needs to increase the temperature $T$ of the bath to a large enough value and decrease the friction coefficient $\eta$ accordingly to keep $\eta T$ invariant. With this efficient method we calculate the efficiency of a three-level heat engine weakly coupled to its heat baths. The result compares well to the prediction of a simple theory for weak coupling limit.

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