Quench of non-Markovian coherence in the deep sub-Ohmic spin-boson model: A unitary equilibration scheme

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The deep sub-Ohmic spin-boson model shows a longstanding non-Markovian coherence at low temperature. Motivating to quench this robust coherence, the thermal effect is unitarily incorporated into the time evolution of the model, which is calculated by the adaptive time-dependent density matrix renormalization group algorithm combined with the orthogonal polynomials theory. Via introducing a unitary heating operator to the bosonic bath, the bath is heated up so that a majority portion of the bosonic excited states is occupied. It is found in this situation the coherence of the spin is quickly quenched even in the coherent regime, in which the non-Markovian feature dominates. With this finding we come up with a novel way to implement the unitary equilibration, the essential term of the eigenstate-thermalization hypothesis, through a short-time evolution of the model.

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I. INTRODUCTION

The molecular materials, both organic and biological, are usually with high degree of dynamic disorder, which induces the strong effect of localization and quantum decoherence. It then seems reasonable to account the intrinsic mechanism of the charge conduction incoherent. However, as widely accepted the transport mechanism in these materials undergoes a transition from coherent to incoherent at finite temperature [1]. Many recent experiments then devoted to uncover the coherent component accordingly [2–5]. For example, the transient absorption spectrum experiment shows an ultrafast charge transfer process following with a long-termly incoherent decay of the population of the induced charge transfer state [2]. These advances of the experiment are deserving the appropriate theoretical explanations, but the present theoretical study lags behind. The significant issue to hinder the progress is that, the decoherence process is not easy to be self-consistently involved in the coherently quantum dynamics [6]. For example, in the dynamic disorder model we have shown that the electron’s coherence can not be quenched by the motion of lattice without any artificial implements of decoherence [7]. Consequently, we are on the stage of thinking about how to smoothly adapt the decoherence into the pure-state quantum dynamics and incorporate the two kinds of mechanisms, coherent and incoherent, into a unified framework.

Our motivation of the present work is based upon the progress of the thermalization emerged in the last several years, which is achieved through a purely quantum-mechanical manner [8–14]. Of the most importance in the field is the eigenstate-thermalization hypothesis (ETH), which states that while evolving, a random initial pure state of the universe, namely the composite of a system plus a bath, produces the same thermal average of the observables of the system [10, 11]. Moreover, another significant statement addresses that a sufficiently small system weakly coupled with a bath always thermalizes no matter how far it is initially from thermal equilibrium [12]. These novel concepts are moving the understanding of the quantum statistical mechanics forward presently. In this context, reexamining the statement in different system-bath coupling models goes active and comprehensive [15–27]. Initially, the adaptive time-dependent density matrix renormalization group (t-DMRG) studies of both one-dimensional spinless fermion and bose-Hubbard model after a quantum quench showed the breakdown of thermalization for both integrable and nonintegrable cases [13, 14]. Soonafter, the exact diagonalization studies gave distinct results for integrable and nonintegrable cases of both one-dimensional boson and fermion models [15]. Following this line, the thermalization and ergodicity are both demonstrated for one-dimensional open systems [9, 10, 18].

By definition, if the ETH holds, the thermalization of an observable of the system is guaranteed for any pure state of the composite with well-defined macroscopic observables [8, 9]. There are three elements to describe this so-called quantum thermalization [12]. (1) If the system (under the influence of bath) initially far from equilibrium always evolves to and remains in a particular state, we call it equilibration. (2) The equilibrated state of the system should be independent of the microscopic details of the initial states of both the system and the bath. (3) In a certain degree, the population of equilibrated state should take the form of Boltzmann distribution. The former two terms

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are attributed to be generic for the quantum thermalization, while the third one calls for a specific coupling term in the Hamiltonian. Our present work is motivated to incorporate the decoherence into the pure-state dynamics, namely to properly involve the influence of bath in the time evolution of the system. So hereafter, we will mainly focus on the equilibration of the system, that is the first two terms of the quantum thermalization.

It has been addressed that the necessary condition of quantum thermalization relies on whether the available space of the bath is large enough such that the coherence of system can be easily quenched \[12\]. Or alternatively speaking, whether the system thermalizes strongly depends on the decoherence induced by the bath \[26, 27\]. So far, several system-bath coupling models have been studied comprehensively for the subject of thermalization. For example, a nine-site Hubbard model, which is numerically exactly solvable, was investigated by considering two sites out of the nine to be the system \[27\]. Here, as we are interested in the transportation mechanisms in molecular materials, the spin-boson model (SBM) will be taken into account. To our knowledge, the study of the quantum thermalization of this model is still absent in the researches up to now. The Hamiltonian of SBM reads \[28, 29\], \((\hbar = 1)\)

\[
H = H_s + \frac{\sigma^z}{2} \sum_l \lambda_l (b_l^\dagger + b_l) + \sum_l \omega_l b_l^\dagger b_l,
\]

where \(H_s = \frac{\varepsilon}{2} \sigma^z - \frac{\Delta}{2} \sigma^x\) is the Hamiltonian for the spin with \(\sigma^z\) and \(\sigma^x\) being the usual notations for Pauli operators, \(\varepsilon\) the bias induced by the external magnetic field, and \(\Delta\) the tunneling constant; \(\lambda_l\) is the coupling constant between the spin and the boson of \(l\)-th mode, \(\omega_l\) the respective frequency, and \(b_l^\dagger (b_l)\) the creation (annihilation) operator of bosons. The degree of freedom of the spin is much smaller than that of bosons, so we can safely recognize the spin as a small system and the bosons as the bath. In addition, the SBM is a highly abstract model to simulate the transportation in molecular materials, such as the excitation energy transfer process \[30\]. The spin represents a two-level system and the bosons simulate the phonon environment. So in principle our study here could be helpful for the understanding of coherent-incoherent transition of transportation in the relevant materials.

The frequency of the boson in SBM is usually cut off at \(\omega_c\), which is chosen to be 1 as unit. The spectral density function of the bath is expressed as \(J(\omega) = 2\pi\alpha\omega_c^{1-\epsilon}\omega^\epsilon\) with \(\alpha\) being the dimensionless spin-boson coupling. The regime \(\epsilon < 1\) refers to the sub-Ohmic bosonic bath showing the strong non-Markovian feature, which is addressed to induce long-term coherence and dominate the dynamics \[31\]. In particular, very recent studies indicated that \[32, 33\], at low temperature there is a persistently coherent regime for deep sub-Ohmic case (\(\epsilon < 0.5\)) so that the spin keeps oscillating during the time evolution. In order to simulate the coherence in the transportation of molecular materials, we will then work in this regime in the present work. Especially, as the robust non-Markovian featured coherence in this regime emerges contradictorily to the decoherence requirement of ETH, it is then available to study the situation that the dynamics of the system loses the coherence (or reaches equilibrated state equivalently) during a short-time quantum evolution.

Consequently, ETH is claimed to be as generic as the concept of thermalization, but the studies of the pure-state dynamics of deep sub-Ohmic SBM shows contradictions to it. In order to solve this seemingly paradoxical problem, in this work, we investigate the quantum dynamics of the model in the coherent regime following the first two requirements of ETH. A steady value of spin population, namely the equilibration, is obtained and the non-Markovian feature is shown to be quickly quenched. The paper is organized as follows. The methodology we use is introduced in Sec. II. Calculation results for both one spin and two spins are presented in Sec. III, where the thermalization and effective temperature are discussed. Conclusions are drawn in the final section.

II. METHODOLOGY

As mentioned above, the necessary condition of thermalization in a quantum-mechanical fashion is, in our opinion, the decoherence time of the system is shorter than the relaxation time. In this situation the quantum coherence of the system could be quickly quenched before the thermalization is achieved. This condition requires that a sufficiently large eigenstate space of the bath has been (or at least could be) occupied \[12\]. However, this is not the case in SBM especially in the coherent regime. Firstly, the strong non-Markovian feature of the bath always gives rise to the longstanding coherence and memory of the initial state. Secondly, based upon the variational theory, during the time evolution, the sub-Ohmic bath could be perfectly described by some combinations of the coherent states \[33\]. The number of these states is not large enough to quench the coherence. Therefore, it is necessary to find a novel way to enlarge the number of available states of the bath.

To this end, we first make a transformation to the Hamiltonian. In the present form of Hamiltonian \([1]\), each bosonic mode of the bath has its own channel to influence the spin, and the coupling in between cannot be regarded to be relatively weak. Alternatively, the theory of orthogonal polynomials presents one way to solve this problem \[34\], \(i.e.,\) to transform the bosonic modes into a one-dimensional chain, with each site in the chain representing a
FIG. 1: (a) Schematic for the effect of heating operator (see definition in the text). Initially, the bath is around the bottom of the potential function (blue point). With the action of heating operator, the potential energy changes, but the configuration of displacement keeps unchanged (red point). Hence, the possible number of states that the bath may occupy increases. (b) The flowchart of the calculating procedure with t-DMRG algorithm. \( |g\rangle \) and \( |h\rangle \) denote the ground state and heated state, respectively.

renormalized mode, and most importantly, the spin interacts with only the first site of the chain. This transformation is exact, via which we are able to make the spin-bath coupling change from nonlocal to local and minimize the action of the bath on the spin. It then becomes available to consider a really “small” system (the spin) embedding in a “large” bath (the bosonic chain). The transformed Hamiltonian is written as

\[
\hat{H} = H_s + \sqrt{\frac{\eta}{4\pi}} \sigma^z (b_1^\dagger + b_1) + \sum_n \omega_n b_n^\dagger b_n + \sum_n (t_n b_{n+1}^\dagger b_n + \text{h.c.}),
\]

where \( \eta \) is the renormalized spin-boson coupling, which could be estimated by \( \eta = \int \omega c_0 J(\omega) \, d\omega \); \( n \) represents the \( n \)-th renormalized mode (bosonic site), and \( \omega_n \) and \( t_n \) are the respective transformed frequency and hopping integral among \( n \) and \( n + 1 \) site, whose precise expressions could be found in Ref. \( 34, 35 \). On each site, the dimension of the Fock space must be cut off at some finite number. Our recent work has tested different parameters and compared the results with that from two other approaches \( 35 \). The comparison shows that, the results are reliable when the dimension of the Fock space of each site is cut off at 4. Here we will keep working with the same parameter to make sure the results are credible.

The dynamics based upon Hamiltonian (2) could be calculated by the adaptive time-dependent density matrix renormalization group (t-DMRG) algorithm \( 35 \). The spin and the bosonic sites together form a one-dimensional lattice chain with only nearest-neighbor interaction. The topology of this lattice is friendly for DMRG calculation and we have obtained precise results with DMRG truncating number of 100 \( 35 \). The calculating procedure in this work is divided into three steps. (i) We set \( \varepsilon \) to \(-0.5\) and calculate the ground state \( |g\rangle \) of the Hamiltonian (2). This will make the spin freeze in its up state and the bath almost in its vacuum state. (ii) Based on the calculated ground state \( |g\rangle \), the bath is heated up under the action of the operator \( \mathcal{H} \) described in the next paragraph. (iii) We change \( \varepsilon \) to the desired value and calculate the time evolution of the whole system with the initial state being \( |h\rangle = \mathcal{H} |g\rangle \). The whole procedure is sketched in Fig. (1b) and is based on the concept of pure-state evolution, which is consistent with the premise of ETH.

The central point in the calculating procedure is to appropriately introduce the thermal effect into the bath, i.e., to let the bath initially be with some kind of heated state. Although there have been some temperature-dependent DMRG algorithms \( 36 \), they are both inefficient and impractical for the present model. To this end, we first introduce an operator of the bath, i.e., \( \mathcal{D} = \delta \sum_n (b_n^\dagger + b_n) \), with \( \delta \) being an effective polarization field for each mode. The motivation of this introduction is as follows. As the operator \( \mathcal{D} \) commutes with the coupling term of the Hamiltonian, namely the second term of the right hand side of (2), the action of it does not change the coupling energy with respect to the coupling term. Its effect is only to enhance the energy of the bath itself, which is what we want. Furthermore, in order to minimize the possible error that the operator \( \mathcal{D} \) may bring to the computations, we introduce another operator \( \mathcal{H} = e^{-i\mathcal{D} \tau_H} \) as mentioned above, with \( \tau_H \) the action time of the polarization field onto the bath. This operator is unitary so that we can divide \( \tau_H \) into many time steps and apply \( \mathcal{H} \) to the state calculated by DMRG. The precision of the action of the unitary operator \( \mathcal{H} \) could be well controlled and the results are then highly reliable.
Subsequently, we have introduced two parameters $\delta$ and $t_H$. For simplicity, in the practical computations $\delta$ is set to be unity and the final results are dependent of $t_H$.

To make it clear, Fig. 1(a) shows a schematic of the effect of the introduced operator $\mathcal{H}$. Suppose the bath initially stays at the vacuum state. As the operator $\mathcal{H}$ is acted on the bath itself, the kinetic energy of the bath, or equivalently the internal energy, could be largely increased by its action. In this situation much more bath states could be occupied than the case that the bath is at the bottom of the energy potential. The essential points of the advantage of this adaption are then worth noting. Firstly, as the operator $\mathcal{H}$ does not commute with the momentum operator of bosons, the effect of the operator is to effectively change the kinetic energy of the bosons which makes the motion of bosons dynamically disordered. This effect is equivalent to heating up the bath in a duration of $t_H$, so the operator $\mathcal{H}$ could be regarded as a “heating” operator and $t_H$ the “heating” time. Secondly, as the initial state of the time evolution is a pure state, the unitary heating operator $\mathcal{H}$ will keep the system-bath composite in a pure state. Hence, we are always working with the pure state instead of some mixed state as in many other algorithms, such as the Lindblad master equations [18], the Monte-Carlo based approach [37] and the polaron theory [38].

III. RESULTS AND DISCUSSIONS

In this section, we will mainly discuss our calculating results for the thermalization of deep sub-Ohmic SBM. In particular, as the thermalization proves for the relatively weak coupling case, throughout this work we will focus on the regime of $s = 0.25$ and $\alpha \leq 0.03$ in which the non-Markovian feature is very robust at low temperature.

A. Unitary equilibration of the spin population

We first show in Fig. 2 the dependence of the spin’s up-state population evolution on $t_H$ for $\Delta = 0.1, \varepsilon = 0$ and $\alpha = 0.02$ and 0.03. It is found that when $t_H$ is relatively small, namely $0.2\pi$, the oscillating behavior of the spin is very similar to that at zero temperature ($t_H = 0$), regardless of the coupling strength. This oscillation is dominated...
by the non-Markovian feature of the bath, as frequently discussed in the literature \cite{35}. There is a small shift of the 
amel{amplitude} of spin population in between, which is very similar with that of changing the initial state from factorized to polarized \cite{31}. This comparison indicates that when \( t_H \) is small our heating procedure is actually to make an initial displacement of the bath.

Then we increase \( t_H \) and the situation changes. The oscillation is quickly quenched after several periods, e.g. three periods for \( t_H = 0.3\pi \), two periods for \( t_H = 0.4\pi \), and one period for \( t_H = 0.6\pi \). Especially, when \( t_H \) is increased to 0.6\( \pi \), the up-state population quickly evolves towards a steady value just after one oscillation period. According to the ETH, this is the so-called equilibration. As we have stated, since the heating operator \( \mathcal{H} \) is unitary, the state of the system-bath composite is always a pure state, and due to the strong non-Markovian effect the dynamics of a pure state is traditionally expected to be sensitive to the initial state and keep oscillating for a long time duration \cite{31}. Our results clearly show a way to break this consequence and to quench the non-Markovian feature. To our knowledge, this effect has not been obtained in the coherent regime through a short-time evolution without any non-unitary adaption. Our present results then establish a prototype for the quench of non-Markovian featured coherence in a unitary fashion, which is the essential result of the present work.

In the inset of Fig. \ref{fig:3} (a), we show the \( t_H \) dependence of the bath’s energy with respect to the last two terms of Hamiltonian \cite{24}. \( t_H \) is chosen to be smaller than 0.6\( \pi \) since our numerical method has truncated the Fock space of bosons and restrict the energy in an extent smaller than about 6\( \omega_c \). In the inset of Fig. \ref{fig:3} (b), the relative deviation of the total energy during the time evolution is shown. Ideally it should be vanishing due to the unitarity of our calculating procedure. Here, we find the deviation is always smaller than 1\% which is an acceptable precision for the numerical method.

In Fig. \ref{fig:4} we show the \( \varepsilon \) dependence of equilibrated value of the up-state population for \( t_H = 0.3\pi \). The equilibrated value is obtained when \( \rho_+ \) becomes unchanged after a long time duration (about 300\( \omega_c^{-1} \) for \( t_H = 0.3\pi \)). For \( \varepsilon = 0 \), the equilibrated value of up-state population is 0.5, the expected thermalized value according to the Boltzmann distribution. Following \( \varepsilon \) increases, the equilibrated value of the up-state population goes down, implying the population of higher-energy state decreases. This finding suggests the equilibration has appropriately taken place as expected.

So far, one would be wondering why our method is able to produce the equilibration in a completely unitary manner.
heating the bath to the corresponding energy, we then get a bath with the effective temperature than respect to the last two terms of Hamiltonian (2), and $N$ we realize that all the bath states with energy below $T$ of the bath could be calculated by $\xi$ is defined as $\xi \equiv (\hat{b}^\dagger + \hat{b})/2$. It is shown that, when $t_H$ is small, there are several bosonic sites, whose displacement does not change very much during the time evolution. As we have discussed above, this is very similar with the case of polarized initial state. The reason of the effect is that, the hopping integral in Hamiltonian $H$ decreases with respect to the distance from the spin and those sites far away from the spin hardly participate in the dynamics. On the other hand, however, when $t_H$ is large, more sites are active due to the initial action of heating operator. This comparison tells us that because of the participation of more bosonic sites, much more bosonic states than that in the usual approaches begin to play significant roles in the dynamics, such that the spin dynamics can be damped and the thermalization takes place. This improvement benefits from the action of heating operator, which acts on every bosonic sites and make them working. Consequently, we would like to address that, this approach of activating the bosonic states as many as possible could be generalized to the quantum-classical methods to self-consistently study the transition from coherent to incoherent mechanism.

### B. Effective temperature

As to a generic definition of the thermalization, it is necessary to define a temperature to make sense of the thermal distribution. In a common sense, the usual definition of an effective temperature for the quantum models relies on a sufficiently long-time evolution, during which the system is always expected to evolve to a thermally equilibrated state. But in this work, the heated bath quenches the robust non-Markovian feature and quantum coherence during a short-time duration. In this context one would then wonder whether the heating effect obtained here is equivalent to that based upon the usual definition of temperature. In a generic manner they are not necessarily to be the same, since as mentioned the Boltzmann distribution calls for the specific coupling term in the Hamiltonian and needs to be studied case by case. So in the following let us discuss the present SBM specifically.

In our numerical method, the number of Fock states on each site of the bath has been truncated to 4, so the number of the available bath states in the evolution could be computed although it is extremely large. Fig. 5 shows the relationship between the number of states and the energy of the bath. From this figure, the effective temperature of the bath could be calculated by $T = (\partial \ln N(E_B)/\partial E_B)^{-1}$ with $k_B = 1$, $E_B$ being the energy of the bath with respect to the last two terms of Hamiltonian (2), and $N(E_B)$ being the number of bath states with energy smaller than $E_B$. Here, $N(E_B)$ is calculated by summing up the number of states from 0 to $E_B$. It is cumulative since we realize that all the bath states with energy below $E_B$ are active and playing roles in the evolution. Hence, by heating the bath to the corresponding energy, we then get a bath with the effective temperature $T$ defined here. The inset of Fig. 2(a) has shown the relationship between the energy of the bath $E_B$ and the heating time $t_H$. Combined with Fig. 5, the relationship between $t_H$ and the effective temperature $T$ could then be established quantitatively. In particular, for $s = 0.25$ and $\alpha = 0.02$, the value $t_H = 0.2\pi$ is found to be equivalent to the effective temperature $T \simeq 0.1\omega_c$, $t_H = 0.3\pi$ to $T \simeq 0.6\omega_c$, $t_H = 0.4\pi$ to $T \simeq 2.5\omega_c$ and $t_H = 0.6\pi$ to $T \simeq 5.6\omega_c$.

Before ending this subsection, we discuss more about the thermal distribution. For the Boltzmann distribution function we can define a formula $\exp(-W/2T)$ with $W = \sqrt{\varepsilon^2 + \Delta^2}$ being the energy difference between the spin’s eigen-energies depending on both the $\varepsilon$ and $\Delta$. But in the SBM we study the coupling term involves the operator $\sigma^z$, namely the preferred spin states of the bath are almost the up- and down-state on $z$ orientation. This implies...
that the equilibrated spin population might be more dependent of the bias $\varepsilon$, so the equilibrated up-state population versus the $\varepsilon$ shown in Fig. 3 could be a good reference of the validness of thermal distribution in the SBM. However, a rigorous verification needs a lot of computations which is out of the scope of the present work.

C. Quench of entanglement

To further convince the unitary equilibration we should compare our results with that from the mixed-state based approach. It has been found qualitatively by the benchmarking quasidiabatic propagator path integral (QUAPI) [37] that at finite temperature the quantum entanglement between two spins in a common bath induced by the non-Markovian feature will be completely quenched. In order to see whether our pure-state evolution could give rise to the similar effect, it is necessary to involve two spins 1 and 2 in the Hamiltonian (2). Namely, the Hamiltonian of spin $H_s$ is replaced by

$$H'_s = \sum_{\mu=1,2} \frac{\varepsilon}{2} \sigma_\mu^z - \sum_{\mu=1,2} \frac{\Delta}{2} \sigma_\mu^x + J \sigma_1 \cdot \sigma_2,$$

where $J$ being the exchange constant between the spins and $\sigma_{1,2}$ the Pauli operator for spin 1 and 2, respectively. The coupling terms between the respective spin with the common bath take the same formula as that in (2). The parameters in the new Hamiltonian are chosen as $\varepsilon = 0, \Delta = 0.05$ and $J = 0.1$ such that the system is initially in an entangled state. The exchange constant $J$ is large enough to induce a strong entanglement between the two spins. Then the bath is heated by the heating operator $\mathcal{H}$ via the same procedure described above. Starting with the heated state we calculate the time evolution of the entanglement between the two spins which is measured by the concurrence. The calculating procedure of the time evolution is the same with that in our preceding work [35].

In Fig. 6 we show the results for various $t_H$ and $\alpha = 0.02$. We can find that when $t_H$ is small, namely the bath’s energy is low, the entanglement evolution shows an oscillating behavior for a long duration. Following the $t_H$ increases the entanglement decreases and when $t_H = 0.4\pi$ the effect of entanglement sudden death and revival appears. We further increase the $t_H$ to $0.6\pi$, the entanglement is completely quenched in a very short duration ($\omega_c t < 50$). In a quantum-mechanical manner, the oscillation, sudden death and revival of entanglement are clearly signatures of the non-Markovian behavior. With increasing $t_H$ these features are gradually suppressed and finally completely quenched. Notice that different from the quench of the oscillation behavior for one-spin case, the entanglement here is not completely quenched within the duration $\omega_c t < 300$ for $t_H = 0.3\pi$ and $0.4\pi$. This is simply because the time scale of the two-spin system is different from that of one-spin system. Subsequently, we would like to indicate that the quench of the non-Markovian features in two-spin system is still closely related to the unitary equilibration as we discussed above. It also helps us to make sense of the unitary equilibration in the non-Markovian dominated SBM.

IV. CONCLUSION

In summary, we have investigated the thermodynamics of the deep sub-Ohmic spin-boson model. A heating operator is introduced, whose action is to enhance the energy of the bosonic bath without changing the coupling energy. Via this operation, the bath is heated up to an effective temperature and the dynamics of the spin embedding in the heated
bath is intensively discussed. The equilibration is found to take place regardless of the coupling strength and the non-Markovian behavior induced by the bath is shown to be quickly quenched. Consequently, we have presented an applicable way to study the unitary equilibration of the deep sub-Ohmic SBM. Especially, our study suggests a novel way to quench the quantum coherence in the dynamics in molecular materials, that is, to let as many as possible bath states to participate in the time evolution. This conclusion is generalizable for the subjects of coherent-incoherent transition. In addition, the method we develop could also be applied to many other related subjects, such as the heat current transmission through a spin sandwiched in two heated bosonic baths.

Acknowledgments

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