



Quantum entanglement and the Born-Markov approximation for an open quantum system

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We revisit the Born-Markov approximation for an open quantum system by considering a microscopic model of the bath, namely, the Bose-Hubbard chain in the parameter region where it is chaotic in the sense of quantum chaos. It is shown that strong ergodic properties of the bath justify all approximations required for deriving the Markovian master equation from the first principles.

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I. INTRODUCTION

Nowadays one witnesses a renewed of interest in open quantum systems, with the emphasis shifted to open many-body systems [1–8]. The standard approach to dynamics of an open system is the master equation for the reduced density matrix,

$$\rho_S(t) = \text{Tr}_B[R(t)], \quad (1)$$

where $R(t)$ is the total density operator of the combined system consisting of the system of interest (subindex S) and the bath (subindex B). In the Markovian case, the dynamics of the matrix $\rho_S(t)$ is governed by the Lindblad equation [9–12],

$$\begin{aligned} \frac{d\rho_S}{dt} = & -i[H_S, \rho_S] \\ & - \sum_n \frac{\gamma_n}{2} (\rho_S V_n^\dagger V_n - 2V_n \rho_S V_n^\dagger + V_n^\dagger V_n \rho_S), \end{aligned} \quad (2)$$

where H_S is the system Hamiltonian and γ_n and V_n are some relaxation constants and operators. Mathematically, this structure of the master equation is fixed by the condition of positivity for the density matrix [13]. However, the microscopic derivation of Eq. (2) is a tedious procedure which involves a number of approximations. These approximations, known as the Born-Markov approximation, are usually summarized as follows.

(i) Interaction between the system and the bath is weak enough that one can neglect the back action of the system on the bath.

(ii) Correlation time for the relevant bath observables is much shorter than the characteristic timescale of the system dynamics.

(iii) The system and the bath are uncorrelated; i.e., at any time the total density matrix factorizes into the tensor product of the reduced density matrices,

$$R(t) = \rho_B(t) \otimes \rho_S(t). \quad (3)$$

Although the listed assumptions formally allow one to derive the master equation (2), they have not been checked for any realistic model of the bath. In this work we fill this gap in the theory by considering a simple microscopic “system + bath” model. We simulate the full dynamic of this

combined system and show that the assumption (3) actually never holds because of the onset of quantum entanglement between the system and the bath. The analysis of this entanglement, which is one of the aims of this work, is given in Sec. III, after introducing the model in Sec. II. We also analyze the correlation time of the relevant bath observables in Sec. IV and relate it to the spectrum and eigenstate statistics of the bath. These results help us to identify the conditions under which the Markovian approximation for the system of interest is justified. Finally, in Sec. V we discuss the conceptual problem related to the assumption (3). It is argued that this (invalid) assumption can be substituted by a weaker assumption which still suffices to derive the master equation (2) but does not assume the absence of correlation between the system and the bath.

II. THE MODEL

We consider a two-level system, $H_S = \delta\hat{\sigma}_z$, which is attached to the first site of the Bose-Hubbard chain,

$$H_B = -\frac{J}{2} \sum_{l=1}^{L-1} (\hat{a}_{l+1}^\dagger \hat{a}_l + \text{H.c.}) + \frac{U}{2} \sum_{l=1}^L \hat{n}_l (\hat{n}_l - 1). \quad (4)$$

The latter system is known to be generally chaotic in the sense of quantum chaos [14–16] that is reflected in the Wigner-Dyson spectrum statistics and ergodic properties of the eigenstates [17,18]. As the coupling operator we choose

$$H_{\text{int}} = \epsilon (\hat{a}_1^\dagger \hat{a}_2 \hat{\sigma}_+ + \text{H.c.}). \quad (5)$$

Thus, the “spin” flips up if a Bose particle tunnels into the first site of the chain and flips down if the particle tunnels out of this site.

We also assume that H_B is in a highly excited state. Then one may expect that it acts as an infinite-temperature bath which equilibrates the population of the system energy levels. In terms of the master equation, this would correspond to the relaxation operator

$$\begin{aligned} \mathcal{L}(\rho_S) = & -\frac{\gamma_1}{2} (\rho_S \hat{\sigma}_+ \hat{\sigma}_- - 2\hat{\sigma}_- \rho_S \hat{\sigma}_+ + \hat{\sigma}_+ \hat{\sigma}_- \rho_S) \\ & -\frac{\gamma_2}{2} (\rho_S \hat{\sigma}_- \hat{\sigma}_+ - 2\hat{\sigma}_+ \rho_S \hat{\sigma}_- + \hat{\sigma}_- \hat{\sigma}_+ \rho_S), \end{aligned} \quad (6)$$

where $\gamma_1 = \gamma_2$.

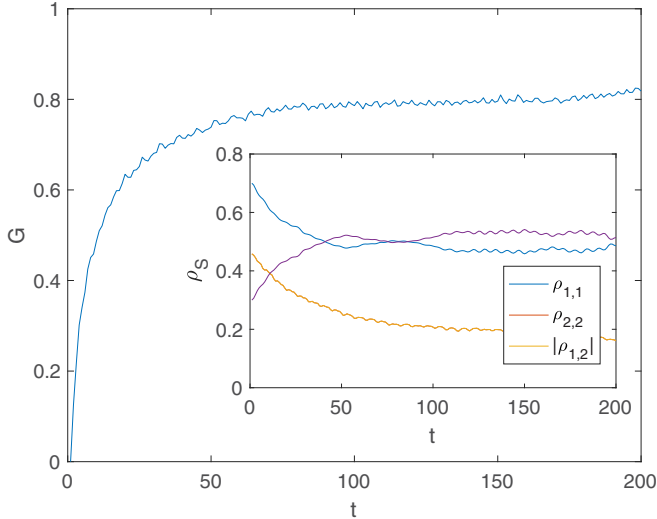


FIG. 1. Main panel: The quantity (8) as the function of time. Inset: The matrix elements of the reduced density matrix $\rho_S(t)$. The system parameters are $\delta = 0.5$ and $\epsilon = 0.2$. The bath parameters are $J = 1$, $U = 0.8$, $N = 6$, and $L = 7$. The initial bath state is given by the eigenstate of the Bose-Hubbard Hamiltonian with the energy $E = 2.8361$.

III. SYSTEM DYNAMICS

First we illustrate the invalidity of Eq. (3). We simulate the dynamics of the total system,

$$R(t) = W(t)R(0)W^\dagger(t),$$

$$W(t) = \exp(-iHt), \quad H = H_S + H_B + H_{\text{int}}, \quad (7)$$

for the initial condition given by a product state, i.e., $R(t=0) = \rho_B \otimes \rho_S$. Although the uncorrelated initial state is usually considered to be a rather important assumption for validity of the master equation, here we use it exclusively to demonstrate the onset of quantum entanglement. To be certain we choose $\rho_S = |\psi\rangle\langle\psi|$, where $|\psi\rangle$ is given by a coherent superposition of the two system eigenstates, $|\psi\rangle = \sqrt{0.7}|\uparrow\rangle + \sqrt{0.3}|\downarrow\rangle$ and $\rho_B = |\Psi\rangle\langle\Psi|$, where $|\Psi\rangle$ is an eigenstate of the Bose-Hubbard Hamiltonian with the energy $E = \langle\Psi|H_B|\Psi\rangle$ from the central part of its energy spectrum [see Fig. 3(a) below]. In this case the Bose-Hubbard chain acts as a high-temperature bath, inducing relaxation of the reduced density matrix $\rho_S(t)$ into a diagonal matrix (see inset in Fig. 1). The decay of the off-diagonal elements reflects the onset of entanglement between the system and the bath which we characterize by the quantity

$$G(t) = \frac{|R(t) - \rho_B(t) \otimes \rho_S(t)|}{|R(t)|}, \quad (8)$$

where the modulus sign denotes the sum of all matrix elements taken by the absolute value. (Another measure of entanglement based on the information entropy is discussed in Appendix A.) A rapid growth of entanglement is clearly seen in Fig. 1. We mention that time fluctuations of the matrix elements of $\rho_S(t)$ can be greatly reduced by choosing a few eigenstates in a narrow energy interval as the initial bath state, i.e., $\rho_B(t=0) \sim \sum_j |\Psi_j\rangle\langle\Psi_j|$. This additional average also

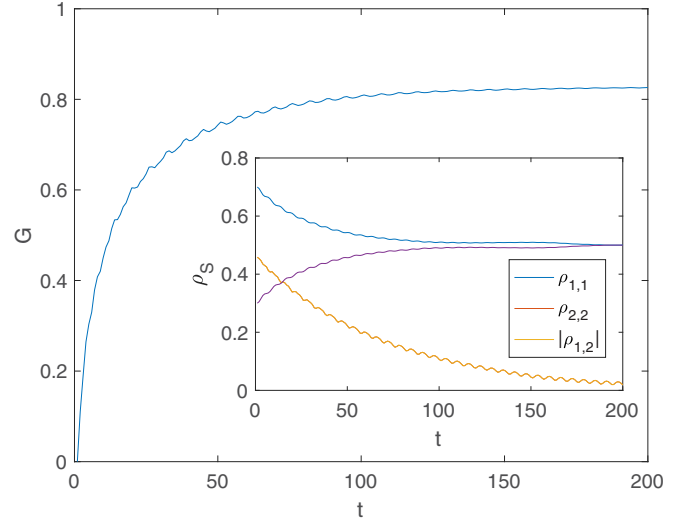


FIG. 2. The same as in Fig. 1 yet for the initial bath state $\rho_B(t=0) \sim \sum_j |\Psi_j\rangle\langle\Psi_j|$ where the sum is taken over 100 eigenstates falling in the energy interval $2.45 \leq E \leq 3.21$.

reveals the exponential law for the decay of the off-diagonal elements with the decay rate proportional to ϵ^2 (see Fig. 2).

A comment on the value of the coupling constant ϵ is in turn. As it was mentioned in the introductory part of the paper, ϵ has to be small to justify the Markovian master equation (2). However, since we work with a finite bath, it must not be smaller than some critical value ϵ_{cr} . One finds this critical value by analyzing the spectrum statistics of the total Hamiltonian. Figure 3(b) shows the integrated level-spacing distribution for the parameters of Fig. 1, yet $\epsilon = 0$, where it is given by the direct sum of two independent Gaussian orthogonal ensemble (GOE) spectra. When ϵ is increased from zero to ϵ_{cr} the level-spacing distribution converges to

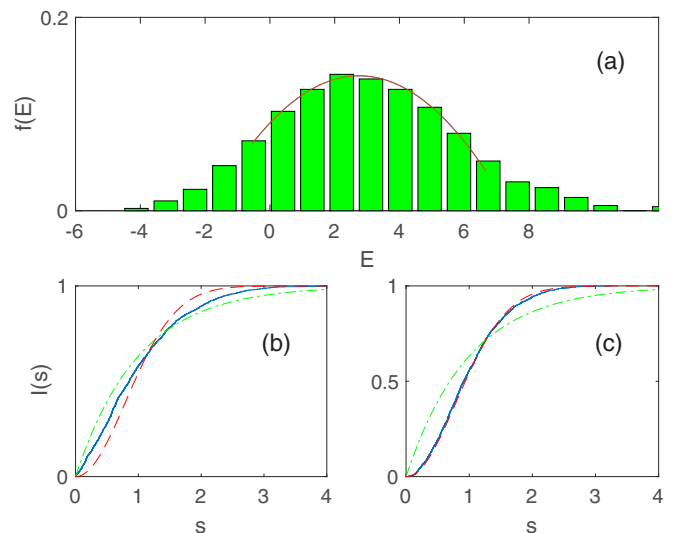


FIG. 3. Lower panels: Integrated level-spacing distribution for the (unfolded) energy spectrum of the total Hamiltonian H for $\epsilon = 0$ (b) and $\epsilon = 0.2$ (c). Notice that small ϵ does not affect the density of state shown in panel (a).

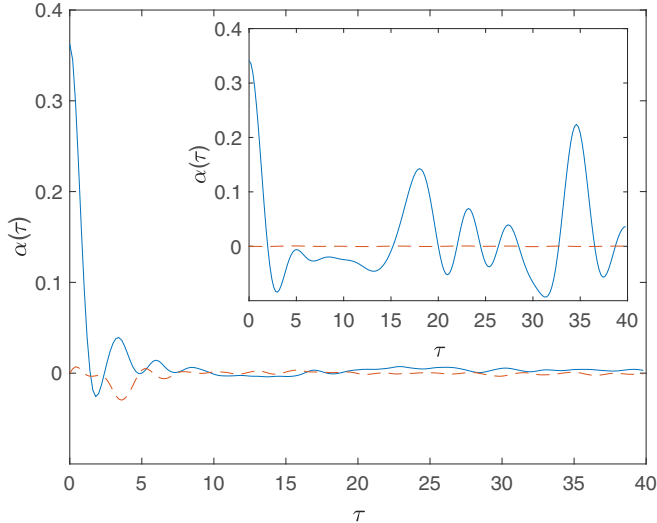


FIG. 4. Main panel: The real (solid line) and imaginary (dashed line) parts of the correlation function (9) as the function of τ at $t = 100$. Parameters are the same as in Fig. 2. Inset: Correlation function of the regular bath which is obtained by setting $U = 0$ in the Bose-Hubbard Hamiltonian.

that for a single GOE spectrum [see Fig. 3(c)]. Remarkably, the critical ϵ decreases with an increase of the bath size. For example, $\epsilon_{\text{cr}} = 0.2$ for $(N, L) = (5, 6)$ (dimension of the bath Hilbert space $\mathcal{N}_B = 504$), $\epsilon_{\text{cr}} = 0.1$ for $(N, L) = (6, 7)$ ($\mathcal{N}_B = 924$), and $\epsilon_{\text{cr}} \leq 0.05$ for $(N, L) = (7, 8)$ ($\mathcal{N}_B = 3432$). Thus, the existence of the lower boundary for the coupling constant is a finite-size effect.

IV. BATH CORRELATION TIME

Next we discuss the correlation time of the bath. The relevant to the master equation correlation function of the bath has the form

$$\alpha(\tau, t) = \text{Tr}_B[\Lambda(\tau)\rho_B(t)],$$

$$\Lambda(\tau) = \exp(-iH_B\tau)\hat{a}_1^\dagger\hat{a}_2\exp(iH_B\tau)\hat{a}_2^\dagger\hat{a}_1. \quad (9)$$

The function $\alpha(\tau, t)$ is shown in Fig. 4, where we fixed time to $t = 100$. It is seen in Fig. 4 that correlations decay within the characteristic time $\tau^* \approx 4$, which is short enough compared to the characteristic timescale of the system dynamics shown in Fig. 2.

We stress that the decay of correlations is entirely due to the chaotic nature of the bath. For the sake of comparison the inset in Fig. 4 shows the correlation function for $U = 0$ where the Bose-Hubbard model reduces to L linear oscillators. We also mention that for chosen $t = 100$ the system and the bath are already strongly entangled so that $\rho_B(t = 100)$ principally differs from $\rho_B(t = 0)$. Yet, we get the same result if we choose $t = 0$. This clarifies the meaning of the statement that one can neglect back action of the system on the bath—it does not imply that $\rho_B(t) \approx \rho_B(0)$ but that the ergodic properties of the bath remain unchanged. A formal proof of this statement as well as a more detailed analysis of the correlation function based on the statistics of the transition matrix elements of the interaction Hamiltonian H_{int} is given in Appendix B.

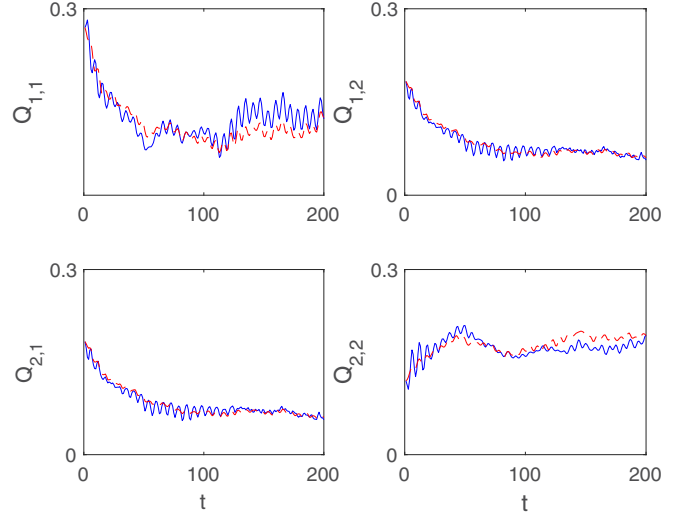


FIG. 5. Four quantities calculated according to the left-hand side (solid lines) and the right-hand side (dashed lines) of Eq. (10).

V. ENTANGLED VS UNCORRELATED

As it was demonstrated in Sec. III, the assumption (3), which is explicitly or implicitly used in every tutorial on the master equation, never holds. Fortunately, one can justify a weaker than Eq. (3) assumption, namely,

$$\text{Tr}_B[\Lambda R(t)] = \text{Tr}_B[\Lambda\rho_B(t)]\rho_S(t), \quad (10)$$

where Λ is an arbitrary operator defined in the bath Hilbert space [19]. It is easy to see that Eq. (10) formally follows from Eq. (3), but the opposite is not true. Nevertheless, Eq. (10) together with the assumptions (i) and (ii) suffices to derive the master equation (2).

We check the validity of Eq. (10) numerically, where as the operator Λ we consider $\Lambda(\tau = 0) = \hat{a}_1^\dagger\hat{a}_2\hat{a}_2^\dagger\hat{a}_1$. The solid and dashed lines in four panels in Fig. 5 show four quantities calculated according to the left-hand side and the right-hand side of Eq. (10). A reasonable agreement is noticed. It should be stressed that the discussed equation is not mathematically exact and may hold only with some accuracy. Originally it was deduced in Ref. [19] by appealing to the mixing property of classical chaotic systems and the quantum-classical correspondence. The result in Fig. 5 indicates that this equation also holds in the case where the quantum system has no obvious classical counterpart.

VI. CONCLUSION

To summarize, we considered the microscopic model of the bath given by the Bose-Hubbard model in the parameter region where it is chaotic in the sense of quantum chaos. Unlike the other, most popular microscopic model of the bath—an infinite number of linear oscillators—the chaotic Bose-Hubbard bath has strong ergodic properties that lead to wide-scale quantum entanglement not only between the bath modes but also between the bath modes and the system of interest which is coupled to the bath. It was shown that these ergodic properties justify all assumptions which one needs to

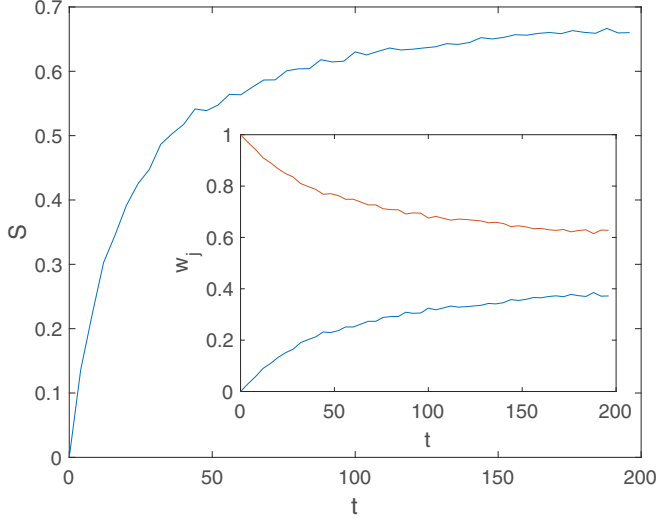


FIG. 6. Von Neumann entropy, main panel, and eigenvalues of $\rho_S(t)$, inset, as the function of time for the parameters of Fig. 1.

derive the Markovian master equation for the reduced density matrix of the system.

As the final remark we mention that the considered microscopic model of the bath also allows us to study other situations and problems. In particular, choosing the energy of the initial bath state in the left slope of its density of states will mimic a finite-temperature bath where $\gamma_2 < \gamma_1$ in Eq. (6). Besides this one can address the case of a non-Markovian bath by decreasing the interaction constant U in the Bose-Hubbard Hamiltonian to the value where it is partially chaotic. We reserve these problems for future studies.

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APPENDIX A

For the initial condition used in Fig. 1 the total density matrix $R(t)$ is a pure state for any time. However, the reduced density matrices $\rho_S(t)$ and $\rho_B(t)$ become mixed states in the course of time. Using the spectral decomposition we have

$$\rho_S(t) = \sum_{n=1}^2 w_n(t) |\phi_n(t)\rangle \langle \phi_n(t)|, \quad (\text{A1})$$

where $w_n(t)$ and $|\phi_n(t)\rangle$ are eigenvalues and eigenstates of the 2×2 matrix $\rho_S(t)$. The commonly accepted quantitative characteristic of the entanglement is the information entropy $S(t) = -\sum_n w_n \log(w_n)$. The dynamics of the entropy $S(t)$ and eigenvalues $w_n(t)$ are exemplified in Fig. 6.

Analogously, for the reduced density matrix of the bath we have

$$\rho_B(t) = \sum_{n=1}^{\mathcal{N}_B} w_n(t) |\Phi_n(t)\rangle \langle \Phi_n(t)|, \quad (\text{A2})$$

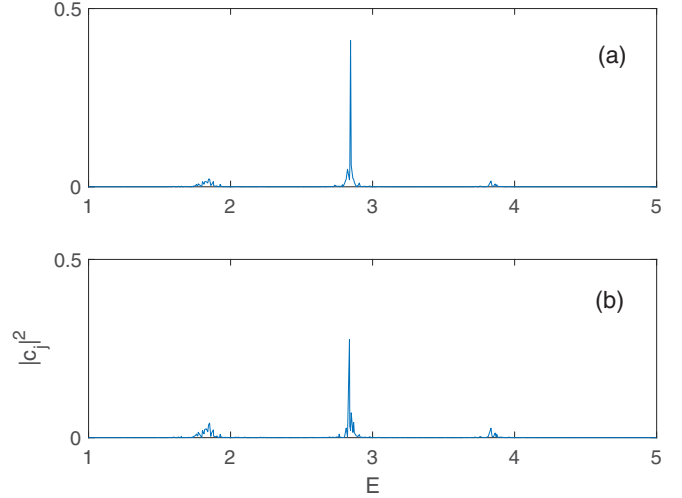


FIG. 7. Expansion coefficients $c_j^{(n)}(t)$ by squared modulus of the states $|\Phi_1(t)\rangle$, panel (a), and $|\Phi_2(t)\rangle$, panel (b), at $t = 200$.

where the summation formally runs to \mathcal{N}_B —the dimension of the Hilbert space of the Bose-Hubbard Hamiltonian. However, according to the Schmidt theorem for the pure $R(t)$ only two eigenvalues $w_n(t)$ differ from zero, and they coincide with the eigenvalues of $\rho_S(t)$. Thus, the information entropy of the bath is the same. The difference appears in the structure of the eigenstates. Figure 7 shows the expansion coefficients of the states $|\Phi_1(t)\rangle$ and $|\Phi_2(t)\rangle$ in the bath energy basis,

$$|\Phi_n(t)\rangle = \sum_{j=1}^{\mathcal{N}_B} c_j^{(n)}(t) |\Psi_j\rangle. \quad (\text{A3})$$

It is seen that the system-bath interaction admixes to the initial bath state $|\Psi_E\rangle$ with the energy $E = 2.8361$ the other eigenstates of H_B which form three groups separated by the energy interval 2δ . Since δ is assumed to be small compared to the width of the bath spectrum, all these states have the same ergodic properties as the initial state. This implies, in particular, that the mean value of any observable, $\langle \Lambda \rangle = \langle \Psi_j | \Lambda | \Psi_j \rangle$, is the same up to statistical fluctuations. Thus,

$$\text{Tr}[\Lambda \rho_B(t)] = \text{Tr}[\Lambda \rho_B(t=0)]. \quad (\text{A4})$$

This equation can be viewed as a formalization of the statement about the negligible effect of the system on the bath. The result (A4) can be easily generalized to the case where the initial bath state is a mixed state. Notice, however, that in this case the von Neumann entropies of the system and the bath are different.

APPENDIX B

The shape of the correlation function in Fig. 4 is determined by the statistics of the transition matrix elements of the interaction Hamiltonian. In fact, in terms of the eigenstates and eigenenergies of the Hamiltonian H_B , Eq. (9) can be

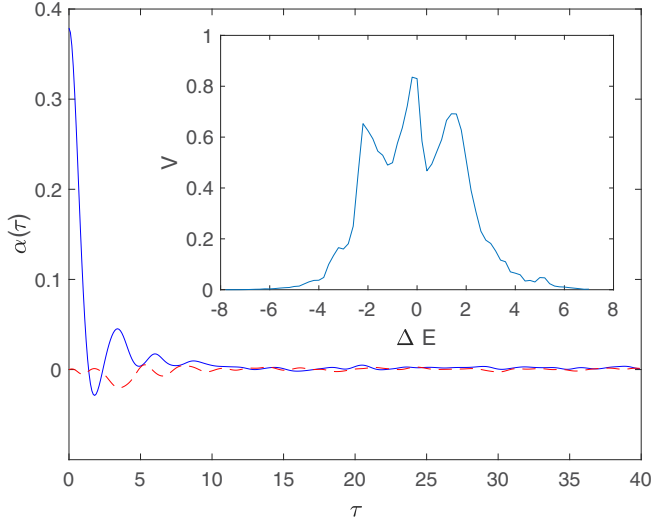


FIG. 8. Main panel: The correlation function of the bath calculated according to Eq. (B1). Inset: Distribution function for the transition matrix elements. To reduce statistical fluctuations, here we consider a larger bath $(N, L) = (7, 8)$ where the dimension of the bath Hilbert space is $\mathcal{N}_B = 3432$.

written as

$$\alpha(\tau) = \sum_k |\langle \Psi_k | \hat{a}_1^\dagger \hat{a}_2 | \Psi_j \rangle|^2 e^{i(E_k - E_j)\tau}, \quad (\text{B1})$$

where we set $t = 0$ and $|\Psi_j\rangle$ is the initial bath state. Labeling the states $|\Psi_k\rangle$ by their energies instead of the index k , Eq. (B1) takes the form

$$\alpha(\tau) = \int dE V(E, E_j) e^{i(E - E_j)\tau}, \quad (\text{B2})$$

where

$$V(E, E_j) = \overline{|\langle \Psi_k | \hat{a}_1^\dagger \hat{a}_2 | \Psi_j \rangle|^2} \quad (\text{B3})$$

and the bar denotes the average over a small energy interval dE . Notice that the function (B3) depends only on the energy difference $\Delta E = E - E_j$. Thus, we have an additional average over E_j if the initial bath state is a mixed state.

The function $V = V(\Delta E)$ is depicted in the inset in Fig. 8. It is a structured Gaussian where the number and positions of local peaks are determined by the value of the interaction constant U . This fine structure of $V(\Delta E)$ is responsible for oscillations of $\alpha(\tau)$, whereas the Gaussian envelope determines the overall decay of the correlation function as

$$\alpha(\tau) \sim \exp \left[- \left(\frac{\tau}{\tau^*} \right)^2 \right], \quad (\text{B4})$$

where the correlation time τ^* is inversely proportional to the Gaussian width.

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