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# Properties of a macroscopic system as a thermal bath

Alberto Suárez and Robert Silbey

Department of Chemistry, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139

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A macroscopic system acting as a heat reservoir affords a simplified description in terms of a collection of independent modes. Although in most cases this model is unable to account for the behavior of the macroscopic system itself, it provides a consistent description of the macroscopic degrees of freedom acting as a dissipation mechanism for a microscopic system. This is found to be a consequence of the statistical properties of bath quantities relevant to the dynamics of the microscopic system. Furthermore, these properties ensure that the unphysical features of the independent bath model do not affect its performance as a heat reservoir.

## I. INTRODUCTION

The case study of a small system in interaction with a macroscopic system which acts as a heat reservoir has been one of the most ubiquitous models for irreversible processes in both classical and quantum mechanics.<sup>1-8</sup> Irreversibility emerges from microscopically reversible equations in the thermodynamic limit, and should be understood as a statement about the behavior of reduced quantities, associated with a small number of degrees of freedom.

In general, it is assumed that the relaxation of a system coupled to dissipative degrees of freedom is largely independent of the specific nature of the bath. The only differentiating features can be ascribed to the spectrum of the bath, which should be continuous, and the strength of the coupling. In particular, the usual assumption is that the necessary information for relaxation is contained in the spectral function.

The heat bath is then modeled by a collection of independent modes (elementary excitations). This choice is particularly convenient from a computational point of view: By eliminating the bath degrees of freedom, the reduced dynamics for the system variables can be obtained. Then, the expressions for the irreversible decay of these variables to their equilibrium values can be evaluated analytically, provided that we choose a mathematically tractable model for the heat bath, such as independent modes.

Despite the mathematical advantages of this treatment, we note that it presents several unphysical features. In particular, the presence of the coupling between the elementary excitations is necessary in order that the isolated bath equilibrate: If the modes are truly independent, energy cannot be transferred from one mode to the others, and equilibrium is never achieved. On the other hand, there exist collective properties of the bath that may critically depend on the interaction between modes.

The question we address in the present investigation is whether the independent mode bath can reproduce the features of a physical one, despite the aforementioned drawbacks. The answer turns out to be related to the statistical properties of the system-bath coupling in the thermodynamic limit, which we shall show to be independent of the nature of the macroscopic system acting as a heat reservoir.

In Sec. II, we shall analyze a Hamiltonian for a system interacting with  $N$  independent modes via a coupling term  $V$ . It is argued that the effect of this coupling should be independent of  $N$ , in order that the problem be well-defined in the limit  $N \rightarrow \infty$ . This restriction on the order of  $V$  with respect to  $N$  has important consequences in the calculation of thermal (canonical ensemble) averages of analytic functions of  $V$ . In Sec. III, we make use of the statistical properties discussed in Sec. II in order to obtain the reduced dynamics of the system in simple cases. These exactly solvable models are employed to illustrate two issues which are of great relevance to the theory of relaxation: The role of constants of motion of the bath, and the equivalence between different models for the bath. The latter point shall be established through comparison between a bath of harmonic oscillators and a bath of two-level systems. Finally, Sec. IV shall be devoted to the derivation of a perturbative solution for the reduced dynamics of the system, in the weak coupling case ( $V$  is small). This derivation serves to expose the general validity of the conclusions obtained in Sec. III through the investigation of simple examples.

## II. MODEL HAMILTONIAN: STATISTICAL PROPERTIES

In this section, we shall analyze a class of Hamiltonians that has been used to describe the interaction of a small system with a heat reservoir. The dynamics of the isolated system are generated by  $H_s$ , which operates on an  $n$ -dimensional Hilbert space, where  $n$  is a small number. Its spectral decomposition is  $H_s = \sum_i E_i |i\rangle\langle i|$ . The macroscopic bath shall be modeled by  $H_b$ , which is not necessarily the true Hamiltonian for the isolated bath, as discussed in the Introduction (it should be sufficient that  $H_b$  yields a good approximation for the true spectrum). In particular, we shall choose  $H_b = \sum_{\alpha=1}^N H_\alpha$ , i.e., the Hamiltonian for a collection of independent modes  $\alpha = 1, \dots, N$ .  $H_b$  has a spectral decomposition of the form

$$H_b = \sum_n E_n |\underline{n}\rangle\langle\underline{n}|,$$

where  $|\underline{n}\rangle \equiv |n_1\rangle \otimes |n_2\rangle \otimes \cdots \otimes |n_N\rangle$  with  $H_\alpha |n_\alpha\rangle = E_{n_\alpha} |n_\alpha\rangle$  and  $E_{\underline{n}} = \sum_{\alpha=1}^N E_{n_\alpha}$ . Finally, the coupling term

$V$ , contains operators of the system and the bath. The complete Hamiltonian is

$$H = H_s + H_b + V. \quad (1)$$

As stressed before, we shall be interested in the reduced dynamics of the system (the dissipative variables are eliminated by taking the trace over them), in the thermodynamic limit:  $N \rightarrow \infty$ .

We note that in this limit, the bath energy scales as  $N$ , whereas the system observables scale as  $N^0$ . This imposes a restriction upon  $V$ , whose effect should be of order  $N^0$  in order that the problem be well posed in the thermodynamic limit. From this formal restriction,  $V$  can be shown to have a series of statistical properties which are universal (in the sense that they do not depend on the choice for  $H_s$ ).

In particular, consider the operator

$$\hat{O} = \sum_{\alpha=1}^N a_{\alpha} \hat{O}_{\alpha},$$

where  $\hat{O}_{\alpha}$  is a Hermitian operator acting upon the Hilbert space corresponding to the  $\alpha$ th mode of the bath. The quantities that are going to be relevant in relaxation theory are ensemble averages of analytic functions of  $\hat{O}$ :

$$\langle \hat{O} \rangle = \sum_n g_n \langle \underline{n} | \hat{O} | \underline{n} \rangle. \quad (2)$$

We shall be interested in canonical ensemble averages, at a temperature  $T$ :

$$g_n = \exp(-\beta E_n)/Z,$$

$$Z = \sum_n \exp(-\beta E_n),$$

where  $Z$  is the canonical ensemble partition function.

We shall then require that  $\langle f(\hat{O}) \rangle$  be of order  $N^0$ , where  $f$  is an analytic function of  $\hat{O}$  [i.e.,  $f(\hat{O}) = \sum_k f_k \hat{O}^k$ ]. There are two cases that should be handled separately, which are described in Secs. II A and II B.

### A. $\langle \hat{O} \rangle = \sum_{\alpha=1}^N a_{\alpha} \langle \hat{O}_{\alpha} \rangle \neq 0$

In this case, the requirement  $\langle f(\hat{O}) \rangle \sim N^0$  when  $N \rightarrow \infty$  implies that  $a_{\alpha} \sim N^{-1}$ , which leads to the identity

$$\langle f(\hat{O}) \rangle = f(\langle \hat{O} \rangle). \quad (3)$$

This can be proved by examining the cumulant expansion of the ensemble average  $\langle \exp(x\hat{O}) \rangle$ :

$$\begin{aligned} \log \langle \exp(x\hat{O}) \rangle &= \log \left\langle \exp \left( x \sum_{\alpha=1}^N a_{\alpha} \hat{O}_{\alpha} \right) \right\rangle \\ &= \log \left\langle \prod_{\alpha=1}^N \exp(xa_{\alpha} \hat{O}_{\alpha}) \right\rangle \\ &= \sum_{\alpha=1}^N \log \langle \exp(xa_{\alpha} \hat{O}_{\alpha}) \rangle \\ &= \sum_{\alpha=1}^N \log [1 + xa_{\alpha} \langle \hat{O}_{\alpha} \rangle + \mathcal{O}(a_{\alpha}^2)] \end{aligned}$$

$$\begin{aligned} &= x \sum_{\alpha=1}^N a_{\alpha} \langle \hat{O}_{\alpha} \rangle + \mathcal{O}(N^{-1}) \\ &= x \langle \hat{O} \rangle + \mathcal{O}(N^{-1}). \end{aligned}$$

Therefore in the thermodynamic limit,

$$\langle \exp(x\hat{O}) \rangle = \exp(x\langle \hat{O} \rangle)$$

for all values of  $x \in \mathcal{C}$ , where  $\mathcal{C}$  is the set of complex numbers. This implies

$$\langle \hat{O}^n \rangle = \langle \hat{O} \rangle^n.$$

### B. $\langle \hat{O} \rangle = 0$

From the hermiticity of  $\hat{O}$ , we must have

$$\langle \hat{O}^2 \rangle = \sum_{\alpha=1}^N a_{\alpha}^2 \langle \hat{O}_{\alpha}^2 \rangle \neq 0$$

implying that  $a_{\alpha}^2 \sim N^{-1}$ , so that  $\langle f(\hat{O}) \rangle$  be of order  $N^0$ . This leads to the identity

$$\langle f(\hat{O}) \rangle = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dz e^{-z^2} f((2\langle \hat{O}^2 \rangle)^{1/2} z).$$

The proof for this final expression is as follows. Consider

$$\begin{aligned} \log \langle \exp(x\hat{O}) \rangle &= \sum_{\alpha=1}^N \log \langle \exp(xa_{\alpha} \hat{O}_{\alpha}) \rangle \\ &= \log [1 + \frac{1}{2} x^2 a_{\alpha}^2 \langle \hat{O}_{\alpha}^2 \rangle + \mathcal{O}(a_{\alpha}^3)] \\ &= \frac{1}{2} x^2 \sum_{\alpha=1}^N a_{\alpha}^2 \langle \hat{O}_{\alpha}^2 \rangle + \mathcal{O}(N^{-1/2}) \\ &= \frac{1}{2} x^2 \langle \hat{O}^2 \rangle + \mathcal{O}(N^{-1/2}). \end{aligned}$$

Thus in the limit  $N \rightarrow \infty$ ,

$$\langle \exp(x\hat{O}) \rangle = \exp(\frac{1}{2} x^2 \langle \hat{O}^2 \rangle),$$

which implies

$$\langle \hat{O}^{2n} \rangle = (2n-1)!!$$

$$\langle \hat{O}^{(2n+1)} \rangle = 0, \quad n = 0, 1, \dots$$

As  $f(\hat{O})$  is an analytic function of  $\hat{O}$ ,

$$\begin{aligned} \langle f(\hat{O}) \rangle &= \sum_k f_k \langle \hat{O}^k \rangle = \sum_m f_{2m} \langle \hat{O}^{2m} \rangle \\ &= \sum_m f_{2m} \frac{(2m-1)!!}{2^{m/2}} [(2\langle \hat{O}^2 \rangle)^{1/2}]^m \\ &= \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dz \sum_k f_k [(2\langle \hat{O}^2 \rangle)^{1/2} z]^k \exp(-z^2) \\ &= \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dz f[(2\langle \hat{O}^2 \rangle)^{1/2} z] \exp(-z^2). \end{aligned}$$

In the following sections we shall illustrate the consequences of the properties derived above by studying several examples. First, we shall concentrate on exactly solvable models and later a perturbative result shall be given for the weak-coupling case ( $V$  small).

### III. EXACTLY SOLVABLE MODELS

#### A. Role of the constants of motion

One of the unphysical properties of the independent mode bath is that the energy for each of the modes is a conserved quantity (classically this would imply that the system is integrable); only the system-bath interaction can cause these to be time varying. This is clearly the reason for the inability of such a bath to reach equilibrium by the exchange of energy amongst its degrees of freedom. The set of constants of motion is

$$\{\mathbf{1}_b, \{H_\alpha\}_{\alpha=1}^N, \{H_\alpha^2\}_{\alpha=1}^N, \dots\},$$

where  $\mathbf{1}_b$  is the unity operator on the Hilbert space of the bath modes. In order to elucidate the role of projections of the system bath coupling onto this set, we shall concentrate in solving the dynamics for the very simplified Hamiltonian

$$H = H_s + H_b + V,$$

where  $V$  is a constant of motion for the bath; that is,  $V$  has no explicit time dependence and  $[H_b, V] = 0$ . For simplicity, we shall also assume  $[H_s, V] = 0$ , which renders the solution trivial. The case  $[H_s, V] \neq 0$  leads to the same conclusions.

The formal solution for the time dependence of the density matrix is of the form

$$\rho(t) = e^{-iHt}\rho(0)e^{iHt} = e^{-iH^X t}\rho(0), \quad (4)$$

where  $H^X$  is defined by  $H^X O \equiv [H, O]$ . We shall assume that the bath is initially in equilibrium at a temperature  $T$ , and that there exist no correlations with the state of the system (factorization assumption):

$$\rho(0) = \rho_b^{\text{eq}}\sigma(0), \quad (5)$$

where  $\sigma(t) = \text{Tr}_b\rho(t)$  is the reduced density matrix for the system, obtained by taking the trace of the total density matrix over the bath degrees of freedom, and  $\rho_b^{\text{eq}}$  is the equilibrium density matrix for the bath at temperature  $T$ :

$$\rho_b^{\text{eq}} = e^{-\beta H_b}/\text{Tr}_b e^{-\beta H_b}.$$

After inserting the initial conditions [Eq. (5)], Eq. (4) becomes

$$\rho(t) = e^{-iH^X t}\rho_b^{\text{eq}}\sigma(0).$$

From this expression, we can obtain  $\sigma(t)$  by taking the trace over the bath

$$\sigma(t) = \langle e^{-iH^X t} \rangle \sigma(0),$$

where  $\langle \cdots \rangle = \text{Tr}_b(\cdots \rho_b^{\text{eq}})$ . Using the facts that  $[H_b, V] = 0$  and  $[H_s, V] = 0$

$$\sigma(t) = e^{-iH^X t} \langle e^{-iV^X t} \rangle \sigma(0)$$

and taking matrix elements of  $\sigma$  between eigenstates of the system, we obtain

$$\sigma_{ij}(t) = e^{-i\omega_{ij}t} \langle e^{-i[V]_{ij}t} \rangle \sigma_{ij}(0), \quad (6)$$

where

$$\sigma_{ij}(t) = \langle i|\sigma(t)|j\rangle, \quad \omega_{ij} = E_i - E_j$$

and

$$[V]_{ij} = \langle i|V|i\rangle - \langle j|V|j\rangle.$$

In order to evaluate the term  $\langle e^{-i[V]_{ij}t} \rangle$ , the following form shall be chosen for  $V$ :

$$V = f(\Phi), \quad \Phi = \sum_{\alpha=1}^N a_\alpha V_\alpha.$$

In the case where  $\langle V_\alpha \rangle \neq 0$ ,  $a_\alpha \sim N^{-1}$ , the solution is given by

$$\sigma_{ij}(t) = e^{-i\omega_{ij}t} e^{-i\langle V \rangle_{ij}t} \sigma_{ij}(0).$$

Note that the effect of the coupling is just a shift in the system frequencies. The reduced dynamics can be thought as generated by an effective Hamiltonian of the form

$$H_{\text{eff}} = H_s + \langle V \rangle + H_b.$$

The remainder of the system-bath interaction  $\Delta H = H - H_{\text{eff}} = V - \langle V \rangle$  gives rise to corrections that are negligible in the thermodynamic limit.

In the case  $\langle V_\alpha \rangle = 0$ ,  $a_\alpha \sim N^{-1/2}$ , the answer is

$$\sigma_{ij}(t) = e^{-i\omega_{ij}t} \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dz e^{-z^2} \times \exp\{-if[(2\langle [\Phi]_{ij}^2 \rangle)^{1/2}z]t\} \sigma_{ij}(0),$$

leading to decay for the off-diagonal terms ( $i \neq j$ ), which is faster or equal to  $1/\lambda t$  as  $\lambda t \rightarrow \infty$  (by the generalized Riemann-Lebesgue lemma). In particular, if  $f(x)$  has a extremum at  $x = a$ ,  $a \in \mathbb{C}$  (the set of complex numbers), the decay is asymptotic to  $c \times \exp[if(a)\lambda t]/\lambda t$ , where  $c$  is a constant. On the other hand, if  $f(x) = x$ , the decay is Gaussian:

$$\sigma_{ij}(t) = e^{-i\omega_{ij}t} e^{-(1/2)\langle [\Phi]_{ij}^2 \rangle t^2} \sigma_{ij}(0).$$

This form of a perturbation that has projections onto constants of motion of the bath but zero thermal average is rather unique. We have not been able to find a physical interaction that satisfies this condition; hence, we shall not be concerned any further with this kind of coupling.

The main conclusion of this section is that the only constant of motion of the bath that may have a finite effect on the reduced dynamics of the system is  $\mathbf{1}_b$ , as illustrated by the fact that in the physically realisable case, the total Hamiltonian can be replaced by an effective one which has no projections onto the set of constants of motion orthogonal to  $\mathbf{1}_b$ :

$$[(H_\alpha^n - \langle H_\alpha^n \rangle)_{\alpha=1}^N]_{n=1}^\infty.$$

We conclude that the projections of the system bath coupling onto this set has a negligible effect in the limit  $N \rightarrow \infty$ . Hence, the unphysical fact that the model used for the isolated bath does not reach equilibrium by exchange of energy among its modes does not affect the relaxation of a small system coupled to it. The action of a macroscopic system as a heat reservoir is related to the dispersion provided by the continuous spectrum of the bath, and does not require that the macroscopic system be statistical in nature (in the sense that it is better described by a temperature, than by a set of quantum numbers).

## B. Model for pure dephasing

As a further illustration of the consequences of the statistical properties of the system-bath coupling, we shall carry out a reanalysis of the results obtained by Skinner and Hsu.<sup>1</sup> In their investigation on pure dephasing, a model Hamiltonian of the form given by Eq. (1) was proposed, and solved exactly for the particular case of a two-level system coupled to a bath of harmonic oscillators:

$$\begin{aligned} H_s &= w_0 |1\rangle\langle 1|, \\ H_b &= \sum_{\alpha=1}^N w_\alpha \left( b_\alpha^\dagger b_\alpha + \frac{1}{2} \right), \\ V &= \Delta |1\rangle\langle 1|, \end{aligned} \quad (7)$$

where  $\Delta = a\Phi + (W/2)\Phi^2$ ,  $\Phi = \sum_{\alpha=1}^N a_\alpha (b_\alpha^\dagger + b_\alpha)$ , and the decomposition of unity for the two-level system is given by  $|1\rangle = |0\rangle\langle 0| + |1\rangle\langle 1|$ . Note that here  $[H_b, V] \neq 0$ . We shall show that the results of their derivation is valid for a more general case, in which

$$H_b = \sum_{\alpha=1}^N H_\alpha, \quad \Phi = \sum_{\alpha=1}^N a_\alpha V_\alpha, \quad \text{and} \quad \Delta = a\Phi + \frac{W}{2}\Phi^2 \quad (8)$$

with  $\langle V_\alpha \rangle = 0$  that is,  $a_\alpha \sim N^{-1/2}$ .

The solution for the reduced density matrix of the system, assuming  $\rho(0) = \rho_b^{\text{eq}}\sigma(0)$ , is given by

$$\begin{aligned} \sigma(t) &= e^{-iH_s^X t} \text{Tr}_b (e^{-i\int_0^t \hat{V}(\tau) d\tau} \sigma(0) \rho_b^{\text{eq}} e^{i\int_0^t \hat{V}(\tau) d\tau}) \\ &= e^{-iH_s^X t} \langle e_{T_+}^{-i\int_0^t \hat{V}(\tau) d\tau} \rangle \sigma(0), \end{aligned} \quad (9)$$

where  $T_+$  is the time-ordering operator that rearranges the functions on which it operates in such a way that time increases from right to left,  $T_+ T_- = 1$ , and  $\hat{V}(\tau) = e^{iH_b \tau} V e^{-iH_b \tau}$  is written in the interaction representation with respect to the bath Hamiltonian.

Taking the (1,0) matrix element in the basis of eigenstates of the system Hamiltonian,

$$\begin{aligned} \sigma_{10}(t) &= e^{-iw_0 t} \langle e_{T_+}^{-i\int_0^t \hat{\Delta}(\tau) d\tau} \rangle \sigma_{10}(0), \\ \hat{\Delta}(\tau) &= e^{(iH_b \tau)} \Delta e^{(-iH_b \tau)}. \end{aligned}$$

The term  $\langle e_{T_+}^{-i\int_0^t \hat{\Delta}(\tau) d\tau} \rangle$  is evaluated by cumulant expansion.<sup>5</sup> Skinner and Hsu<sup>1</sup> made use of the fact that the variables in  $\Phi$  are Gaussianly distributed (Wick's theorem) to derive analytic expressions for all the cumulants. However, this property holds even in the case that the bath is not a collection of harmonic oscillators. Let us illustrate this point by evaluating a correlation function of the form

$$\begin{aligned} &\langle T_+ \Phi(t_1) \Phi(t_2) \rangle \\ &= \sum_{\alpha\beta\gamma\delta} a_\alpha a_\beta a_\gamma a_\delta \langle T_+ V_\alpha(t_1) \\ &\quad \times V_\beta(t_1) V_\gamma(t_2) V_\delta(t_2) \rangle \\ &= \sum_{\alpha\beta} a_\alpha^2 a_\beta^2 [\langle V_\alpha^2 \rangle \langle V_\beta^2 \rangle + 2 \langle T_+ V_\alpha(t_1) V_\alpha(t_2) \rangle \\ &\quad \times \langle T_+ V_\beta(t_1) V_\beta(t_2) \rangle] \end{aligned}$$

$$\begin{aligned} &+ \sum_\alpha a_\alpha^4 [\langle T_+ V_\alpha^2(t_1) V_\alpha^2(t_2) \rangle \\ &- \langle V_\alpha^2 \rangle^2 - 2 \langle T_+ V_\alpha(t_1) V_\alpha(t_2) \rangle^2] \\ &= \sum_{\alpha\beta} a_\alpha^2 a_\beta^2 [\langle V_\alpha^2 \rangle \langle V_\beta^2 \rangle + 2 \langle T_+ V_\alpha(t_1) V_\alpha(t_2) \rangle \\ &\quad \times \langle T_+ V_\beta(t_1) V_\beta(t_2) \rangle] + \mathcal{O}(N^{-1}) \\ &= \langle \Phi^2 \rangle^2 + 2 \langle T_+ \Phi(t_1) \Phi(t_2) \rangle^2 + \mathcal{O}(N^{-1}) \\ &= C^2(0) + 2C^2(t_1 - t_2) + \mathcal{O}(N^{-1}) \end{aligned}$$

with the definition  $C(t_1 - t_2) \equiv \langle T_+ \Phi(t_1) \Phi(t_2) \rangle$ .

Using this property (for the details of the derivation, we refer to the original paper by Skinner and Hsu), the final result is

$$\sigma_{10}(t) = e^{-iw_0 t} e^{-i\Delta w t} e^{-t/T_2}, \quad (11)$$

where  $\Delta w = \text{Im}\{K\}$ ,  $T_2^{-1} = \text{Re}\{K\}$ , and

$$\begin{aligned} K &= \frac{1}{2} a^2 \widehat{C}(0) [1 + iW\widehat{C}(0)]^{-1} \\ &\quad + \frac{1}{2\pi} \int_0^\infty dw \log[1 + iW\widehat{C}(w)] \end{aligned}$$

and  $\widehat{C}(w)$  is the Fourier transform of  $C(t)$ :

$$\widehat{C}(w) = \int_{-\infty}^\infty dt e^{iwt} C(t).$$

We remark that this expression is valid for any independent mode bath of the specified form [Eq. (8)]. The only difference enters in the evaluation of  $C(t)$  with different models. In order to clarify this point, let us examine the form of  $C(t)$  for two different types of bath.

### 1. Harmonic oscillators bath

The bath Hamiltonian is

$$H_b = \sum_{\alpha=1}^N w_\alpha (b_\alpha^\dagger b_\alpha + \frac{1}{2})$$

and the perturbation is  $\Delta(\Phi)$ , with

$$\Phi = \sum_{\alpha=1}^N a_\alpha (b_\alpha^\dagger + b_\alpha).$$

The result for  $C(t)$  is

$$C^{\text{HO}}(t) = \sum_{\alpha=1}^N \frac{a_\alpha^2}{\exp(\beta w_\alpha) - 1} (e^{\beta w_\alpha} e^{iw_\alpha|t|} + e^{-iw_\alpha|t|}).$$

In the limit  $N \rightarrow \infty$ , the spectrum of the bath becomes continuous and the summation becomes an integral:

$$C^{\text{HO}}(t) = \int_{-\infty}^\infty dw \frac{\Gamma^{\text{HO}}(w)}{\exp(\beta w) - 1} (e^{\beta w} e^{iw|t|} + e^{-iw|t|}), \quad (12)$$

where the definition  $\Gamma(w) = \sum_{\alpha=1}^N a_\alpha^2 \delta(w - w_\alpha)$  has been used.

### 2. Two-level systems bath

For this case

$$H_b = \sum_{\alpha=1}^N w_\alpha \sigma_z^\alpha$$

and

$$\Phi = \sum_{\alpha=1}^N a_{\alpha} \sigma_{\alpha}^{\alpha},$$

where  $\{\sigma_i\}_{i=x,y,z}$  are the Pauli spin matrices, which leads to the result

$$C^{\text{TLS}}(t) = \sum_{\alpha=1}^N \frac{a_{\alpha}^2}{\exp(\beta w_{\alpha}) + 1} (e^{\beta w_{\alpha}} e^{iw_{\alpha}|t|} + e^{-iw_{\alpha}|t|}),$$

which in the continuous limit becomes

$$C^{\text{TLS}}(t) = \int_{-\infty}^{\infty} dw \frac{\Gamma^{\text{TLS}}(w)}{\exp(\beta w) + 1} (e^{\beta w} e^{iw|t|} + e^{-iw|t|}) \quad (13)$$

with the same definition of  $\Gamma(w)$  as earlier.

The remarkable feature of the expressions (12) and (13) is that they are almost identical except for factors that can be absorbed in the spectral function. We conclude that a more useful definition of the spectral function is given by a combination of the form

$$\Gamma(w) = \sum_{\alpha=1}^N \Theta_{\alpha} a_{\alpha}^2 \delta(w - w_{\alpha}), \quad (14)$$

where  $\Theta_{\alpha}$  yields information about specific features of the bath, i.e., the equilibrium distribution is included in its definition.

#### IV. WEAK COUPLING

In the limit that the coupling between the system and the heat bath is weak, the elements of the reduced density matrix of the system can be shown to obey a set of first order coupled linear differential equations, which are local in time (Redfield equations).<sup>3,6</sup> The only requirements for these equations to be valid is that the coupling parameter  $\lambda$  be small, and that time correlation functions for the bath factorize in a time scale  $\tau_b$  much shorter than the characteristic time scale for the system relaxation  $\tau_R \sim \lambda^{-2}$ ; that is,

$$\langle \hat{O}_1(t) \hat{O}_2 \rangle \rightarrow \langle \hat{O}_1 \rangle \langle \hat{O}_2 \rangle \quad \text{for } t \gg \tau_b,$$

where  $\hat{O}_1, \hat{O}_2$  are bath operators, and  $\langle \dots \rangle$  is the canonical ensemble (thermal) average. However, if  $\hat{O}_1$  and/or  $\hat{O}_2$  have projections onto the set of constants of motion of the bath that do not vanish in the thermodynamic limit, the latter condition cannot be fulfilled. Hence, constants of motion of the bath have to be handled separately, as their role is very different from the remainder of the system-bath coupling. This could have been anticipated in view of the properties of the Hamiltonians considered in the preceding sections.

Our objective will be to rederive Redfield equations in the case that the system bath coupling has a projection onto constants of motion:  $V_0 = \sum_{\alpha=1}^N a_{\alpha} V_0^{\alpha}$ . The remainder of the coupling term  $V_1 = \sum_{\alpha=1}^N g_{\alpha} V_1^{\alpha}$  has no diagonal elements in the basis of eigenstates of the bath Hamiltonian  $H = \sum_{\alpha=1}^N H_{\alpha}$ . The total Hamiltonian is

$$H = H_s + H_b + \lambda V_0 + \lambda V_1.$$

It shall be useful to define  $H_0 = H_s + H_b$  and  $\tilde{H}_0 = H_0 + \lambda V_0$ . The formal solution for the total density matrix is

$$\rho(t) = e^{-iH^X t} \rho(0)$$

from which we derive

$$\hat{\rho}^{(0)}(t) = e^{-i\tilde{H}_0^X t} \exp_T \left( -i\lambda \int_0^t \hat{V}_1^X(\tau) d\tau \right) \rho(0),$$

where  $\hat{V}_1^X(\tau) = e^{i\tilde{H}_0^X \tau} V_1 e^{-i\tilde{H}_0^X \tau}$  is written in the interaction representation with respect to  $\tilde{H}_0$ , and  $\hat{\rho}^{(0)}(t) = e^{iH_0^X t} \rho(t) e^{-iH_0^X t}$  is in the interaction representation with respect to  $H_0$ . Using the factorization assumption  $\rho(0) = \rho_b^{\text{eq}} \sigma(0)$  and taking the trace over the bath degrees of freedom, we obtain for  $\hat{\sigma}^{(s)}(t)$  the reduced density matrix of the system in the interaction representation with respect to  $H_s$ , to order  $\lambda^2$

$$\begin{aligned} \hat{\sigma}^{(s)}(t) &= \left\langle e^{-i\tilde{H}_0^X t} \exp_T \left( -i\lambda \int_0^t \hat{V}_1^X(\tau) d\tau \right) \right\rangle \sigma(0) \\ &\approx \langle e^{-i\tilde{H}_0^X t} \rangle \left( 1 - \lambda^2 \int_0^t d\tau \int_0^{\tau} d\tau' \langle e^{-i\tilde{H}_0^X \tau} \rangle^{-1} \right. \\ &\quad \times \left. \langle e^{-i\tilde{H}_0^X \tau} \hat{V}_1^X(\tau) \hat{V}_1^X(\tau') \rangle \right) \sigma(0) \\ &\approx \langle e^{-i\tilde{H}_0^X t} \rangle \exp_O \left( -\lambda^2 \int_0^t d\tau \int_0^{\tau} d\tau' \langle e^{-i\tilde{H}_0^X \tau} \rangle^{-1} \right. \\ &\quad \times \left. \langle e^{-i\tilde{H}_0^X \tau} \hat{V}_1^X(\tau) \hat{V}_1^X(\tau') \rangle \right) \sigma(0) \\ &= \langle e^{-i\tilde{H}_0^X t} \rangle \exp_O \left( -\lambda^2 \int_0^t d\tau \int_0^{\tau} d\tau' \langle \hat{V}_1^X(\tau) \right. \\ &\quad \times \left. \hat{V}_1^X(\tau') \rangle + \mathcal{O}(\lambda^3) \right) \sigma(0). \end{aligned}$$

The last step is only correct if  $a_{\alpha} \sim N^{-1}$ , which we shall assume to be the case (see discussion in Sec. II). We note that to order  $\lambda^2$ , the ordering prescription (indicated by the subscript  $O$  in the exponential) is unimportant. However, it shall be useful to choose the partial ordering prescription<sup>8</sup> (POP), which naturally leads to Redfield equations. The POP is such that the time derivative of  $\sigma(t)$  is

$$\begin{aligned} \dot{\sigma}^{(s)}(t) &= \frac{d}{dt} (\log \langle e^{-i\tilde{H}_0^X t} \rangle) \hat{\sigma}^{(s)}(t) - \lambda^2 \langle e^{-i\tilde{H}_0^X t} \rangle \\ &\quad \times \frac{d}{dt} \left( \int_0^t d\tau \int_0^{\tau} d\tau' \langle \hat{V}_1^X(\tau) \hat{V}_1^X(\tau') \rangle \right) \\ &\quad \times \langle e^{-i\tilde{H}_0^X t} \rangle^{-1} \hat{\sigma}^{(s)}(t). \end{aligned}$$

Taking the matrix element between the  $\langle i |, | j \rangle$  eigenstates of the system Hamiltonian,

$$\begin{aligned} \dot{\sigma}_{ij}^{(s)}(t) &= \frac{d}{dt} (\log \langle e^{-i[V_0]_{ij} t} \rangle) \hat{\sigma}_{ij}^{(s)}(t) - \lambda^2 \langle e^{-i[V_0]_{ij} t} \rangle \\ &\quad \times \sum_{klpq} \left( \int_0^t d\tau \langle (\hat{V}_1^X)_{ijkl}(t) (\hat{V}_1^X)_{klpq}(\tau) \rangle \right) \\ &\quad \times \langle e^{-i[V_0]_{pq} t} \rangle^{-1} \hat{\sigma}_{pq}^{(s)}(t) \end{aligned}$$

with the definitions

$$[V_0]_{ij} = \langle i | V_0 | j \rangle - \langle j | V_0 | i \rangle, \quad (15)$$

$$\begin{aligned} \langle e^{-i\lambda [V_0]_{ij} t} \rangle &= e^{-i\lambda \langle [V_0]_{ij} \rangle t}, \\ \langle (\hat{V}_1^X)_{ijkl}(t) (\hat{V}_1^X)_{klpq}(\tau) \rangle &= \langle (\hat{V}_1)_{ik}(t) (\hat{V}_1)_{kp}(\tau) \rangle \delta_{jq} \\ &\quad + \langle (\hat{V}_1)_{ql}(\tau) (\hat{V}_1)_{lj}(t) \rangle \delta_{ip} \\ &\quad - \langle (\hat{V}_1)_{qj}(\tau) (\hat{V}_1)_{ip}(t) \rangle - \langle (\hat{V}_1)_{qj}(t) (\hat{V}_1)_{ip}(\tau) \rangle. \end{aligned} \quad (16)$$

Undoing the interaction representation with respect to the

system Hamiltonian, we finally obtain

$$\begin{aligned} \dot{\sigma}_{ij}(t) &= -i(w_{ij} + \lambda \langle [V_0]_{ij} \rangle) \sigma_{ij}(t) \\ &\quad - \lambda^2 \sum_{pq} \mathcal{R}_{ijpq} \sigma_{pq}(t). \end{aligned} \quad (17)$$

The relaxation tensor elements are

$$\begin{aligned} \mathcal{R}_{ijpq} = \int_0^\infty d\tau \left( \sum_k \left[ e^{-i(w_{kp} + \lambda \langle [V_0]_{kp} \rangle) \tau} \langle (\hat{V}_1^{(b)})_{ik}(\tau) (V_1)_{kp} \rangle \delta_{jq} + e^{-i(w_{qk} + \lambda \langle [V_0]_{qk} \rangle) \tau} \langle (V_1)_{qk} (\hat{V}_1^{(b)})_{kj}(\tau) \rangle \delta_{ip} \right] \right. \\ \left. - e^{-i(w_{qj} + \lambda \langle [V_0]_{qj} \rangle) \tau} \langle (V_1)_{qj} (\hat{V}_1^{(b)})_{ip}(\tau) \rangle - e^{-i(w_{ip} + \lambda \langle [V_0]_{ip} \rangle) \tau} \langle (\hat{V}_1^{(b)})_{qj}(\tau) (V_1)_{ip} \rangle \right), \end{aligned} \quad (18)$$

where  $\hat{V}_1^{(b)}$  indicates that the superscripted operator is in the interaction representation with respect to the bath Hamiltonian. Note as well, that the upper limit of the time integral have been extended to infinity, which assumes that the time-correlation functions of  $V_1$  vanish in a short time scale  $\tau_b$ . This is true, since  $V_1$  has no projections onto the set of constants of motion of the bath.

The set of equations (17) is just Redfield equations<sup>6</sup> with a shift in the system frequencies, due to  $V_0$ , the projection of the system-bath coupling onto the set of constants of motion of the bath. Once more, we reckon that the same equations could have been derived from an effective Hamiltonian:

$$H_{\text{eff}} = H_s + \lambda \langle V_0 \rangle + H_b + \lambda V_1$$

and that the remainder  $\Delta H = H - H_{\text{eff}} = \lambda(V_0 - \langle V_0 \rangle)$  gives rise to corrections negligible in the thermodynamic limit.

## V. CONCLUSIONS

The independent mode bath has been extensively used as a model for a macroscopic system acting as a heat reservoir. This choice for the bath presents the advantage of affording a relatively simple description. In particular, the reduced dynamics of a small system coupled to this type of bath can be obtained analytically; this task would be practically impossible if, more realistically, we included nontrivial coupling between the modes (nontrivial, in the sense that we cannot perform a unitary transformation such that the many body problem is mapped back into a collection of independent modes). It should be noted, however, that this coupling is essential for the bath to attain full equilibration. In the past, some qualitative arguments and *a posteriori* justifications have been given to account for the validity of this model.

The present investigation establishes that the use of the model is justified owing to the particular properties of the system-bath coupling in the thermodynamic limit. The more relevant consequences are the following:

These properties are universal, which accounts for the formal similarities for results obtained with baths of different characteristics. All the information particular to different models can be summarized in the spectral function for the bath:

$$\Gamma(w) = \sum_{\alpha=1}^N a_{\alpha}^2 \Theta_{\alpha} \delta(w - w_{\alpha})$$

which contains information about the spectrum of the bath, the strength of the coupling to the small system ( $a_{\alpha}^2$ ), and a factor  $\Theta_{\alpha}$  depending on the spectrum of the  $\alpha$ th mode of the bath and, possibly, on the statistics (fermionic-bosonic bath).

The overabundance of constants of motion in the bath does not affect the reduced dynamics of the system: The only relevant constant of motion is  $\mathbf{1}_b$ , the unity operator for the bath (which obviously is a constant of motion of the actual bath).

In some way, the results derived are a consequence of a central limit theorem<sup>9</sup> for operators. Due to the fact that the system-bath Hamiltonian is obtained by a scaled addition of a large number of independent operators whose thermal average is zero, the distribution of the resulting operator has to be Gaussian.

Finally, we would like to stress that the results derived in this paper are valid whenever the spectral function has a finite value over a continuous range of frequencies. If the spectral function is strongly peaked at a particular frequency, the arguments made about  $N$  ordering may not be valid. In this case, the interaction with that set of modes should be included in the zeroth-order description of the system (however, in some cases, this will only amount to a renormalization of the system parameters and a weak residual interaction). Among the systems where we may expect these arguments to be valid stands the important case of a localized system in interaction with a condensed phase where the disorder is not too large, so that the modes with which the localized system interacts are delocalized on length scales large compared to the small system.

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