Universality of quantum Brownian motion

Eric Lutz [1] and Hans A. Weidenmüller

Max Planck Institut für Kernphysik, Postfach 103980, 69029 Heidelberg, Germany

Abstract

Are Markovian master equations for quantum Brownian motion independent of model assumptions used in the derivation and, thus, universal? With the aim of answering this question, we use a random band–matrix model for the system–bath interaction to derive Markovian master equations for the time evolution of one–dimensional quantum systems weakly coupled to a heat bath. We study in detail two simple systems, the harmonic oscillator and the two–level system. Our results are in complete agreement with those of earlier models, like the Caldeira–Legget model and, in the large–band limit, with the Agarwal equations (both with and without rotating–wave approximation). This proves the universality of these master equations.

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1   Introduction

The description of the interaction of an open quantum system with its environment is an important problem in quantum physics. If the environment is modeled as a heat bath, the interaction will lead to relaxation and dissipation processes in the quantum system, and to an irreversible approach toward equilibrium [1]. During the last decades, various models of this type have been introduced in different branches of physics and chemistry. Notable examples are the Redfield theory in nuclear magnetic resonance [2], the Oppenheim–Romero-Rochin model in condensed–phase chemical physics [3], the phase–space approach of Agarwal in quantum optics [4,5], and the influence functional method used by Caldeira and Leggett in condensed–matter physics [6]. The Markovian master equations obtained in these approaches have been recently compared in Ref. [7].

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[1] Corresponding Author. Fax: +49 6221 516 605; e-mail: eric.lutz@mpi-hd.mpg.de

The standard model for quantum dissipation (the Caldeira–Leggett model) consists of a quantum system coupled to an infinite set of harmonic oscillators. Caldeira and Leggett have shown that it is always possible to treat the bath as an ensemble of independent oscillators provided the system–bath coupling is weak. These authors also assumed that the coupling is linear in both, the position coordinate of the quantum system and the bath variables. For the quantum system, this choice follows from the requirement that in the classical limit, the friction force should be linear in the velocity. For the bath, the choice was primarily made for computational convenience. To the best of our knowledge, there is no compelling argument for choosing the interaction term linear in the bath coordinates.

It is expected, of course, that the relaxation process described by a master equation should be insensitive to the detailed form of the system–bath interaction. The work reported in the present paper aims at proving this statement. We do so with the help of an alternative model for the interaction. We use an ensemble of random matrices. The ensemble encompasses all forms of system–bath interaction which are linear in the position coordinate of the quantum system, and which respect fundamental symmetries of the problem like time–reversal invariance. The ensemble is characterized by a few parameters which establish the relevant time scales. The Markovian master equations derived in this fashion are then valid for all possible forms of the interaction between quantum system and heat bath, except for a set of measure zero. We find that in the the high–temperature limit, the Markovian master equations derived by Caldeira and Leggett and others are independent of both the specific structure of the bath and of the specific form of the system–bath interaction. This establishes the universality referred to in the title of our paper.

Random–matrix theory (RMT) was originally introduced by Wigner to describe spectral fluctuations of quantum many–body systems such as nuclei and has since been applied successfully in a wide range of other fields such as quantum chaos and disordered mesoscopic systems [8]. To the best of our knowledge, a random–matrix approach to relaxation has been first developed in nuclear physics in the context of deeply inelastic heavy–ion collisions [9]. Since then, related models have been used to describe relaxation of a non–degenerate two–level system [10], dissipation in complex quantum systems [11,12] and, more recently, the dynamics of a simple quantum system in a complex environment [13].

A second motivation for our work relates to the use of random–matrix models in *closed* quantum systems with many degrees of freedom. In such systems, only few degrees of freedom usually command physical interest. We refer to such degrees of freedom (to the remainder) as to the collective (the remaining) degree(s) of freedom, respectively. A case in point is nuclear fission. Here, interest is focussed on the shape degree of freedom, and little attention is

usually paid to the intrinsic degrees of freedom of the fissioning nucleus. In cases like this, the dynamical behavior of the remaining degrees of freedom depends, however, strongly on that of the collective degree of freedom and, therefore, cannot be modeled as a heat bath. The success of RMT in self–bound many–body quantum systems [8] then suggests that we model the remaining degrees of freedom in terms of a suitable random–matrix model. We have in mind an ensemble of random matrices which depends parametrically on the collective degree(s) of freedom. Such an approach has been taken in the papers by Bulgac et al. [12]. Before investigating the consequences of such an idea, it is necessary to study the limiting case where the environment can indeed be modeled as a heat bath, and to ask whether in this case, the heat bath can be replaced by a suitable random–matrix model. Our proof of universality answers this question affirmatively.

The paper is organized as follows. In Section 2, we present the model for system plus bath with emphasis on the statistical properties of the interaction, a random band matrix. An approximate form for the second moment (shown later to be equivalent to the rotating–wave approximation) is introduced. In Section 3 we derive the Markovian master equation for the averaged density operator of the system. The range of validity of this equation is discussed in Section 4. In Sections 5 and 6 we apply our results to the damped harmonic oscillator and the dissipative two–level system, respectively. We obtain a generalized band–width dependent fluctuation–dissipation relation. We show that in the large band–width limit we recover the Agarwal equations (with and without rotating–wave approximation). Conclusions are drawn in Section 7.

2 The model

We study the properties of a small quantum system S coupled via a random interaction to a large environment, considered as a heat bath. The Hamiltonian of the composite system is given by

$$H = H_S \otimes \mathbb{1}_S + \mathbb{1}_B \otimes H_B + Q \otimes V = H_0 + W \tag{1}$$

where H_S describes the system S (for example, a particle moving in a potential or a spin degree of freedom), H_B describes the bath B (the actual form of H_B is not specified) and $W = Q \otimes V$ the system–bath interaction. We denote by $|n\rangle$ ($|a\rangle$) the eigenstates of the system (bath) Hamiltonian with eigenvalues E_n (ε_a, respectively),

$$H_S|n\rangle = E_n|n\rangle \qquad\qquad H_B|a\rangle = \varepsilon_a|a\rangle \ . \tag{2}$$

The product states $|na\rangle$ form a complete set for the composite system. The operator Q acts on the system S, and V is a Gaussian random band matrix

acting on the bath. The first two moments of V are given by

$$\overline{V_{ab}} = 0 \qquad \overline{V_{ab}V_{cd}} = (\delta_{ac}\delta_{bd} + \delta_{ad}\delta_{bc})\overline{V_{ab}}^2 \tag{3}$$

where the matrix V_{ab} respects time–reversal symmetry and has non–zero elements only in a band of width Δ along the diagonal. More specifically, we adopt a form first given in Ref. [9]. This paper also contains a detailed justification of the form of Eq. (4). This form has been widely used later, cf. Ref [12,13].

$$\overline{V_{ab}}^2 = A_0\left[\rho(\varepsilon_a)\rho(\varepsilon_b)\right]^{-\frac{1}{2}} e^{-\frac{(\varepsilon_a-\varepsilon_b)^2}{2\Delta^2}} \ . \tag{4}$$

Here A_0 is the strength of the coupling, $\rho(\varepsilon)$ the density of states of the bath, and Δ the band width. For W, this implies

$$\text{(I)} \quad \overline{W_{ab}^{mn}} = 0 \quad \overline{W_{ab}^{mn}W_{cd}^{pq}} = (\delta_{ac}\delta_{bd} + \delta_{ad}\delta_{bc})Q_{mn}Q_{pq}\overline{V_{ab}}^2 \ . \tag{5}$$

The form of the Hamiltonian (1) is a generalization of the Hamiltonian considered in Ref. [10]. There it was motivated with the remark that in relaxation problems, the process is frequently found to be insensitive to the details of the interaction. One may therefore construct an ensemble of interactions and calculate the average of the observable over this ensemble. We show below that this is indeed the case.

In Eq. (5), only the part of the interaction acting on the bath is modeled as a random matrix. This is physically sensible since only the bath is supposed to be a complex system. We observe that as a consequence, the variance (I) of W has the inconvenient feature of being not symmetric in the variables of both the system and the bath. Therefore, we also consider a symmetrized form (II) of W where the entire interaction behaves as a random matrix. This form may be thought of as an approximation to the full form (I). We show later that form (II) leads to the rotating–wave approximation. It is given by

$$\text{(II)} \quad \overline{W_{ab}^{mn}} = 0 \quad \overline{W_{ab}^{mn}W_{cd}^{pq}} = (\delta_{ac}\delta_{bd}\delta_{mp}\delta_{nq} + \delta_{ad}\delta_{bc}\delta_{mq}\delta_{np})|Q_{mn}|^2\overline{V_{ab}}^2 \ . \tag{6}$$

Let $\hat{\rho}$ be the density operator for system plus bath. The von Neuman equation for $\hat{\rho}$ reads

$$\hat{\rho}(t) = U(t)\hat{\rho}(0)U^\dagger(t) \tag{7}$$

where the time–evolution operator $U(t) = e^{-iHt}$ obeys Dyson's equation

$$U(t) = U_0(t) - i\int_0^t dt_1 U_0(t-t_1)WU(t_1) \tag{8}$$

and where $U_0(t) = e^{-iH_0t}$ denotes the free time–evolution operator. (We put $\hbar = 1$ throughout). We define the reduced operator for the system S by

$\hat{\rho}_S = tr_B[\hat{\rho}]$ where the trace is taken over the bath states. We assume that the interaction is turned on at $t = 0$ and that at that initial time S and B are not correlated. Then

$$\hat{\rho}(0) = \hat{\rho}_S(0) \otimes \hat{\rho}_B(0) \qquad (9)$$

is the product of the initial density operators $\hat{\rho}_S(0)$ and $\hat{\rho}_B(0)$ for system and bath, respectively. We suppose further that at all times $t \geq 0$ the bath is in thermal equilibrium with temperature T,

$$\hat{\rho}_B = \frac{1}{Z} \sum_a e^{-\beta \varepsilon_a} |a\rangle\langle a| \qquad (10)$$

where Z is the canonical partition function and $\beta = (kT)^{-1}$. Expression (10) can be shown (see Appendix A) to be equivalent to

$$\hat{\rho}_B = |a^*\rangle\langle a^*| \qquad \underline{\text{and}} \qquad \rho(\varepsilon) = \rho_0 e^{\beta \varepsilon} \ , \qquad (11)$$

where the state $|a^*\rangle$ is defined by the temperature T.

3 Derivation of the master equation

In this Section we derive a Markovian master equation for $\hat{\rho}_S(t)$. The equation applies provided the coupling between system and bath is weak. More precisely, we use the following assumptions.

i) The time t obeys the inequalities $t_\Delta \ll t \ll t_P$. Here $t_\Delta = 1/\Delta$ is the duration time of a single action of the interaction and t_P is the Poincare recurrence time of the system. This condition is always needed to describe a relaxation process in terms of a transport equation.

ii) For all states $|n\rangle$ and $|b\rangle$, the band width Δ has to satisfy the inequalities $\omega, \gamma \ll \Delta \ll kT$. Here γ is the relaxation constant and ω denotes the mean level spacing of the system S. For the harmonic oscillator, γ is defined in Eq. (38). For other systems, an analogous definition applies. Condition ii) requires weak coupling between bath and system and ensures the validity of the Markov approximation. It also requires the temperature T to be larger than a minimum temperature $kT_m = \Delta$ and may, therefore, also be seen as defining a semiclassical approximation.

These assumptions are discussed in more detail in Section 4.

Because of the stochastic nature of the interaction W, the time–evolution operator (8) and, consequently, the density operator (7) are themselves random variables. We have to calculate their mean values. The averaging procedure

consists in expanding $U(t)$ in Eq. (8) in powers of W (Born series), averaging term by term, and finally summing up the whole series, see Appendix B. We always work in the limit in which the dimension N of the bath matrices tends to infinity. We consistently omit terms of order N^{-1} and smaller.

We illustrate the procedure by calculating the transition probability per unit time. We suppose that S is initially in some eigenstate $|m\rangle$ with $\hat{\rho}_S(0) = |m\rangle\langle m|$, and we ask for the probability to find the system in another state $|n\rangle$ at a later time t. We have

$$
\begin{aligned}
P_n(t) = \langle n|\hat{\rho}_S(t)|n\rangle &= \sum_b \langle nb|\hat{\rho}(t)|nb\rangle \\
&= \sum_b \langle nb|U(t)|ma\rangle\langle ma|U^\dagger(t)|nb\rangle \ .
\end{aligned} \tag{12}
$$

Expanding $U(t)$ and $U^\dagger(t)$ up to first order in W and taking the average (denoted hereafter by a bar), we obtain

$$
\overline{P_n(t)} = \sum_b \overline{|\langle nb|W|ma\rangle|^2} \, 4\left(\frac{sin(E_n + \varepsilon_b - E_m - \varepsilon_a)\frac{t}{2}}{E_n + \varepsilon_b - E_m - \varepsilon_a}\right)^2 \ . \tag{13}
$$

For $t \gg t_\Delta$, the factor $4(sin^2\frac{1}{2}xt)/x^2$ is sharply peaked at $x = 0$ and may be approximated by $2\pi t \delta(x)$. This yields

$$
\overline{P_n(t)} = 2\pi t \sum_b \overline{|\langle nb|W|ma\rangle|^2} \, \delta(E_n + \varepsilon_b - E_m - \varepsilon_a) \ . \tag{14}
$$

The transition probability per unit time is defined as

$$
W_{nm} = \frac{\overline{P_n(t)}}{t} = 2\pi \sum_b \overline{|\langle nb|W|ma\rangle|^2} \, \delta(E_n + \varepsilon_b - E_m - \varepsilon_a) \ . \tag{15}
$$

This is Fermi's Golden Rule.

We turn to the derivation of the master equation. The averaged density operator $\overline{\rho}(t, t')$ for system plus bath obeys the equation

$$
\begin{aligned}
\overline{\rho}(t, t') = {}& \overline{U}(t)\hat{\rho}(0)\overline{U}^\dagger(t') \\
&+ \int_0^t d\tau \int_0^{t'} d\tau' \, \overline{U}(t - \tau)\overline{W\,\overline{\rho}(\tau, \tau')\,W}\,\overline{U}^\dagger(t' - \tau') \ .
\end{aligned} \tag{16}
$$

The averaged time–evolution operator $\overline{U}(t)$ obeys

$$
\overline{U}(t) = U_0(t) + \int_0^t dt_1 \int_0^{t_1} dt_2 \, U_0(t - t_1)\overline{W\, U_0(t_1 - t_2)\,W}\,\overline{U}(t_2) \ . \tag{17}
$$

To obtain an evolution equation for the averaged reduced density operator $\overline{\rho}_S$, we have to (i) solve Eq. (17), (ii) substitute the resulting $\overline{U}(t)$ into Eq. (16), (iii) take the trace over the bath degrees of freedom and (iv) differentiate with respect to time. We shall see that it is not always possible to perform step (i). This is the case, in particular, for the unsymmetrized variance of Eq. (5). Nevertheless, a master equation can still be derived in the weak coupling limit. This is done in the next two Subsections.

3.1 Case (II)

We begin with the simpler case, i.e., with the approximate form (II). In this case, the averaged time–evolution operator $\overline{U}(t)$ is diagonal and reads (see Appendix B, Eq. (B.14))

$$\overline{U}_{nb}(t) = e^{-i(E_n + \varepsilon_b)t - \frac{\Gamma_{nb}}{2}t} \ . \tag{18}$$

The decay width Γ_{nb} is given by Eq. (B.12),

$$\Gamma_{nb} = 2\pi \sum_{n_1 b_1} \overline{|\langle nb|W|n_1 b_1\rangle|^2} \ \delta(E_n + \varepsilon_b - E_{n_1} - \varepsilon_{b_1}) \ . \tag{19}$$

We substitute $\overline{U}(t)$ from Eq. (17) into Eq. (16) and arrive at

$$\sum_b \langle nb|\overline{\rho}(t,t')|nb\rangle = \sum_b e^{-i(E_n+\varepsilon_b)(t-t') - \frac{\Gamma_{nb}}{2}(t+t')} \langle nb|\hat{\rho}(0)|nb\rangle$$
$$+ \int_0^t d\tau \int_0^{t'} d\tau' e^{(-i(E_n+\varepsilon_b)-\frac{\Gamma_{nb}}{2})(t-\tau)}$$
$$\times \sum_{bn_1 b_1} \overline{|\langle nb|W|n_1 b_1\rangle|^2} \langle n_1 b_1|\overline{\rho}(\tau,\tau')|n_1 b_1\rangle e^{(i(E_n+\varepsilon_b)-\frac{\Gamma_{nb}}{2})(t'-\tau')} \ . \tag{20}$$

We take the time derivatives and get

$$\left(\frac{\partial}{\partial t} + \frac{\partial}{\partial t'}\right) \sum_b \langle nb|\overline{\rho}(t,t')|nb\rangle = - \sum_b \Gamma_{nb} \langle nb|\overline{\rho}(t,t')|nb\rangle$$
$$+ \sum_{bn_1 b_1} \overline{|\langle nb|W|n_1 b_1\rangle|^2} \int_{-t}^0 dt_1 e^{(i(E_n+\varepsilon_b)+\frac{\Gamma_{nb}}{2})t_1} \langle n_1 b_1|\overline{\rho}(t+t_1,t')|n_1 b_1\rangle$$
$$+ \sum_{bn_1 b_1} \overline{|\langle nb|W|n_1 b_1\rangle|^2} \int_{-t'}^0 dt_1' e^{(-i(E_n+\varepsilon_b)+\frac{\Gamma_{nb}}{2})t_1'} \langle n_1 b_1|\overline{\rho}(t,t'+t_1')|n_1 b_1\rangle \ . \tag{21}$$

We have put $t_1 = \tau - t$ and $t_1' = \tau' - t'$.

The right–hand side of Eq. (21) is easily interpreted. The first term (the "loss term") corresponds to transitions which *deplete* the state n whereas the two last terms ("gain terms") correspond to transitions which *feed* the state n. The gain terms are non–local in time and, therefore, involve memory effects. In the limit of weak coupling, however, the process becomes Markovian and the memory effects play no role [14]. To see this, we note that for short times (to zeroth order in W), Eq. (16) reduces to

$$\overline{\rho}(t,t') = U_0(t)\hat{\rho}(0)U_0^{\dagger}(t') . \tag{22}$$

We use this form in the gain terms and accordingly approximate $\langle n_1 b_1 | \overline{\rho}(t + t_1, t') | n_1 b_1 \rangle$ by $e^{-i(E_{n_1}+\varepsilon_{b_1})t_1} \langle n_1 b_1 | \overline{\rho}(t,t') | n_1 b_1 \rangle$ and $\langle n_1 b_1 | \overline{\rho}(t, t' + t_1') | n_1 b_1 \rangle$ by $\langle n_1 b_1 | \overline{\rho}(t,t') | n_1 b_1 \rangle e^{i(E_{n_1}+\varepsilon_{b_1})t_1'}$. Setting $t = t'$, we obtain

$$\frac{d}{dt} \sum_b \langle nb|\overline{\rho}(t)|nb\rangle = -\sum_b \Gamma_{nb}\langle nb|\overline{\rho}(t)|nb\rangle$$
$$+ \sum_{bn_1b_1} \overline{|\langle nb|W|n_1b_1\rangle|^2} \langle n_1 b_1|\overline{\rho}(t)|n_1b_1\rangle$$
$$\times \left[\int_{-t}^{0} dt_1 e^{(i(E_n+\varepsilon_b-E_{n_1}-\varepsilon_{b_1})+\frac{\Gamma_{nb}}{2})t_1} + \int_{-t}^{0} dt_1 e^{(-i(E_n+\varepsilon_b-E_{n_1}-\varepsilon_{b_1})+\frac{\Gamma_{nb}}{2})t_1} \right] . \tag{23}$$

Condition ii) implies $\Gamma_{nb} \ll E_n + \varepsilon_b - E_{n_1} - \varepsilon_{b_1}$. Thus, we neglect Γ_{nb} in the integrands. This amounts to replacing $\overline{U}(t)$ by $U_0(t)$. Moreover, for sufficiently large times we have

$$\int_{-t}^{t} dt_1 e^{(i(E_n+\varepsilon_b-E_{n_1}-\varepsilon_{b_1})t_1} \approx 2\pi\delta(E_n+\varepsilon_b-E_{n_1}-\varepsilon_{b_1}) . \tag{24}$$

Hence, Eq. (23) reduces to

$$\frac{d}{dt} \sum_b \langle nb|\overline{\rho}(t)|nb\rangle =$$
$$2\pi \sum_{bn_1b_1} \overline{|\langle nb|W|n_1b_1\rangle|^2}\delta(E_n+\varepsilon_b-E_{n_1}-\varepsilon_{b_1})\langle nb|\overline{\rho}(t)|nb\rangle$$
$$-2\pi \sum_{bn_1b_1} \overline{|\langle nb|W|n_1b_1\rangle|^2}\delta(E_n+\varepsilon_b-E_{n_1}-\varepsilon_{b_1})\langle n_1b_1|\overline{\rho}(t)|n_1b_1\rangle . \tag{25}$$

We have used Eq. (19) for Γ_{nb}. Using Eq. (12) we finally obtain a master equation of the Pauli type,

$$\frac{d\overline{P}_n(t)}{dt} = \sum_{n_1} W_{nn_1} \sum_{b_1} \langle n_1b_1|\overline{\rho}(t)|n_1b_1\rangle - \sum_{n_1} W_{n_1n} \sum_b \langle nb|\overline{\rho}(t)|nb\rangle$$

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$$= \sum_{n_1} W_{nn_1} \overline{P}_{n_1}(t) - \sum_{n_1} W_{n_1n} \overline{P}_n(t) \ . \tag{26}$$

The transition probabilities are given by the Golden Rule expressions (15),

$$W_{nn_1} = 2\pi \sum_b \overline{|\langle nb|W|n_1 b_1\rangle|^2} \delta(E_n + \varepsilon_b - E_{n_1} - \varepsilon_{b_1}) \ ,$$

$$W_{n_1 n} = 2\pi \sum_{b_1} \overline{|\langle nb|W|n_1 b_1\rangle|^2} \delta(E_n + \varepsilon_b - E_{n_1} - \varepsilon_{b_1}) \ . \tag{27}$$

It may seem curious that in the evaluation of the gain term, it is necessary to invoke the Markov approximation while in the loss term, the limit of weak coupling apparently suffices. To explain this fact, we recall that we always work in the limit of infinite matrix dimension N. The loss term in the Pauli master equation is obtained from single–side Wick contractions, symbolically written as $\overline{VV}(\ ):(\ \underline{\ })$ or $(\ ):(\ \underline{\ })\overline{VV}$, whereas the gain term is generated by Wick contractions $\overline{V(\ ):(\ \ )V}$ which connect matrix elements in both amplitudes. Selection among the first type of Wick contractions is affected by both, the limit $N \to \infty$ and the weak–coupling limit. We exemplify this statement by the terms of fourth order, given by the three Wick contractions $V\overline{V}\overline{V}V$, $\overline{V}V\overline{V}V$, and $\overline{V}\overline{V}VV$. The lines indicate which pairs of V's are Wick–contracted. Of the three, the last is neglected because $N \to \infty$ and the second, because of weak coupling. In contradistinction, the form of the gain terms in Eq. (21) is determined entirely by the limit $N \to \infty$. Hence, an additional step is needed to implement the weak–coupling limit.

3.2   Case (I)

For the non–symmetric form (5) of the variance of the interaction, the averaged time–evolution operator is not diagonal in energy representation. Instead, we have

$$\langle nb|\overline{U}(t)|n'b'\rangle = \delta_{bb'}\langle nb|\overline{U}(t)|n'b\rangle \ . \tag{28}$$

Therefore, the matrix elements $\langle nb|\overline{U}(t)|n'b'\rangle$ cannot be given in closed form (see Appendix B). However, the time derivative of these quantities can be obtained explicitly in the limit of weak coupling. This suffices to obtain the master equation. Aside from this difference, the derivation proceeds in complete analogy to that given in the previous Subsection. In analogy to Eq. (20) we obtain

$$\sum_b \langle nb|\overline{\rho}(t,t')|n'b\rangle = \sum_{bn_1n_2} \langle nb|\overline{U}(t)|n_1 b\rangle \langle n_1 b|\hat{\rho}(0)|n_2 b\rangle \langle n_2 b|\overline{U}^\dagger(t')|n'b\rangle$$

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$$\times \int_0^t d\tau \int_0^{t'} d\tau' \sum_{bn_1} \sum_{\substack{n_2 b_2 \\ n_3 n_4}} \langle nb|\overline{U}(t-\tau)|n_1 b\rangle Q_{n_1 n_2} Q_{n_3 n_4} \overline{V_{bb_2}}^2$$

$$\times \langle n_2 b_2|\overline{\rho}(\tau,\tau')|n_3 b_2\rangle \langle n_4 b|\overline{U}^\dagger(t'-\tau')|n'b\rangle . \qquad (29)$$

We take the double time derivative, use Eqs. (B.25) and (B.26) for the time derivative of the time–evolution operator, the Markov approximation in the gain terms, and the identity

$$\int_0^\infty d\tau e^{ix\tau} = iP\frac{1}{x} + \pi\delta(x) . \qquad (30)$$

We neglect the level shift due to the principal–value integral. All this yields the master equation

$$\frac{d}{dt}\langle n|\overline{\rho}_S(t)|n'\rangle = -i\langle n|[H_S, \overline{\rho}_S(t)]|n'\rangle$$

$$-\frac{1}{2}\sum_{n_1 n_2} W^{(1)}_{nn_1 n_1 n_2}\langle n_2|\overline{\rho}_S(t)|n'\rangle - \frac{1}{2}\sum_{n_1 n_2} W^{(2)}_{n_1 n' n_2 n_1}\langle n|\overline{\rho}_S(t)|n_2\rangle$$

$$\frac{1}{2}\sum_{n_1 n_2} W^{(3)}_{nn_1 n_2 n'}\langle n_1|\overline{\rho}_S(t)|n_2\rangle + \frac{1}{2}\sum_{n_1 n_2} W^{(4)}_{nn_1 n_2 n'}\langle n_1|\overline{\rho}_S(t)|n_2\rangle . \qquad (31)$$

We have defined the generalized transition probabilities

$$W^{(1)}_{nn_1 n_1 n_2} = 2\pi \sum_{b_1} Q_{nn_1} Q_{n_1 n_2} \overline{V_{bb_1}}^2 \, \delta(E_{n_2} + \varepsilon_b - E_{n_1} - \varepsilon_{b_1}) ,$$

$$W^{(2)}_{n_1 n' n_2 n_1} = 2\pi \sum_{b_1} Q_{n_1 n'} Q_{n_2 n_1} \overline{V_{bb_1}}^2 \, \delta(E_{n_2} + \varepsilon_b - E_{n_1} - \varepsilon_{b_1}) ,$$

$$W^{(3)}_{nn_1 n_2 n'} = 2\pi \sum_b Q_{nn_1} Q_{n_2 n'} \overline{V_{bb_1}}^2 \, \delta(E_{n_1} + \varepsilon_{b_1} - E_n - \varepsilon_b) ,$$

$$W^{(4)}_{nn_1 n_2 n'} = 2\pi \sum_b Q_{nn_1} Q_{n_2 n'} \overline{V_{bb_1}}^2 \, \delta(E_{n_2} + \varepsilon_{b_1} - E_{n'} - \varepsilon_b) . \qquad (32)$$

4 Discussion: Time Scales

With an eye on the derivation given in the previous Section, we discuss the various time scales appearing in our model. These time scales play an essential role in defining the range of validity of the master equation [14,15].

According to the statistical *ansatz* in Eq. (4), the interaction V connects eigenstates of H_B within an energy interval $\sim \Delta$. Thus, the band width Δ can be

visualized as the average amount of energy exchanged during a single action of V, and $t_\Delta = 1/\Delta$ can be interpreted as the duration time of a single action of V (i.e., the time needed to transfer the energy Δ). A statistical description in terms of a master equation can be valid only for times $t \gg t_\Delta$.

Any dynamical process in a finite–sized system will return (close) to its initial state after a characteristic time, the Poincare recurrence time t_P (in the example of a two–level system, the Poincare time corresponds to the Rabi period $t_P = 2\pi/(E_+ - E_-)$, where $(E_+ - E_-)$ is the energy difference between the two (perturbed) levels). When the bath is much larger than the system, the recurrence time is essentially determined by the mean level spacing D of the bath, $t_P \sim 1/D$. Obviously, t_P tends to infinity with the size of the bath. This is the condition of irreversibility. The inequality $t \ll t_P$ must be fulfilled in order to have relaxation.

The weak–coupling condition ii) requires that the relaxation constant γ be much smaller than the amount Δ of energy transferred during a single action of the interaction, $\gamma \ll \Delta$ (see also Appendix B). This condition has a simple interpretation in terms of the times that correspond to these energies. The relaxation time $t_R = 1/\gamma$ must be much larger than the time $t_\Delta = 1/\Delta$ needed for a single action of V, $t_\Delta \ll t_R$.

There are two time scales which determine the memory time of the heat bath [16,17]: The time t_Δ (the inverse of the frequency cutoff of the bath in the Caldeira-Leggett model) and the time $t_B = 1/kT$. The latter is purely quantum in origin. For high (low) temperature, thermal (quantum) fluctuations dominate and the memory time of the bath is given by t_Δ (by t_B, respectively). A crossover between thermal and quantum fluctuations occurs at the crossover temperature $kT_m = \Delta$. To garantee the validity of the Markov approximation, the temperature must be much larger than the crossover temperature, $\Delta \ll kT$. This condition can be rephrased in terms of length scales: The range of the interaction must be much larger than the thermal de Broglie wavelength of the Brownian particle $\lambda_{dB} = 1/\sqrt{4MkT}$.

5 First Application: Harmonic oscillator

We illustrate our results for the case where the system S is a harmonic oscillator with mass M and frequency ω. The Hamiltonian H_S is given by $H_S = \frac{p^2}{2M} + \frac{1}{2}M\omega^2 x^2$, and the energy spectrum reads $E_n = (n+1/2)\,\omega$, $n = 1, 2, \ldots$. We assume a coupling linear in the position of the system, $Q = x$. We introduce the usual creation and annihilation operators $a^\dagger$ and a. The elements of the matrix W_{ab}^{mn} vanish unless $|m - n| = 1$.

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5.1 Case (II)

The transition probabilities in Eq. (27) are easily evaluated. We use Eq. (6). For times $t \ll t_P$, we can replace the sum over b by an integral and obtain

$$W_{nn_1} = 2\pi \sum_b |Q_{nn_1}|^2 \overline{V_{bb_1}}^2 \delta(E_n + \varepsilon_b - E_{n_1} - \varepsilon_{n_1})$$

$$= 2\pi |Q_{nn_1}|^2 A_0 \int d\varepsilon_b \left[\frac{\rho(\varepsilon_b)}{\rho(\varepsilon_{b_1})}\right]^{\frac{1}{2}} e^{-\frac{(\varepsilon_b - \varepsilon_{b_1})^2}{2\Delta^2}} \delta(E_n + \varepsilon_b - E_{n_1} - \varepsilon_{b_1})$$

$$= 2\pi |Q_{nn_1}|^2 A_0 e^{\frac{\beta}{2}(E_{n_1} - E_n)} e^{-\frac{(E_{n_1} - E_n)^2}{2\Delta^2}} . \tag{33}$$

In the last line, we have used Eq. (11) for the density of states $\rho(\varepsilon)$. We use $Q = x = \sqrt{\frac{1}{2M\omega}}(a + a^\dagger)$ and obtain for the only non–vanishing terms

$$W_{nn-1} = W_0 n e^{-\frac{\beta}{2}\omega} \qquad W_{nn+1} = W_0(n + 1) e^{\frac{\beta}{2}\omega}$$

$$W_{n-1n} = W_0 n e^{\frac{\beta}{2}\omega} \qquad W_{n+1n} = W_0(n + 1) e^{-\frac{\beta}{2}\omega} \tag{34}$$

where

$$W_0 = \frac{A_0 \pi}{M\omega} e^{-\frac{\omega^2}{2\Delta^2}} . \tag{35}$$

The master equation for the damped harmonic oscillator takes the form

$$\dot{P}_n(t) = W_{nn-1} P_{n-1}(t) + W_{nn+1} P_{n+1}(t) - (W_{n-1n} + W_{n+1n}) P_n(t)$$

$$= W_0 e^{\frac{\beta}{2}\omega} \left[(n + 1) P_{n+1}(t) - n P_n(t)\right]$$

$$+ W_0 e^{-\frac{\beta}{2}\omega} \left[n P_{n-1}(t) - (n + 1) P_n(t)\right] \tag{36}$$

or, equivalently,

$$\dot{P}_n(t) = 2\gamma(n_{th} + 1) \left[(n + 1) P_{n+1}(t) - n P_n(t)\right]$$

$$+ 2\gamma n_{th} \left[n P_{n-1}(t) - (n + 1) P_n(t)\right] \tag{37}$$

where we have defined the relaxation constant

$$2\gamma = W_0(e^{\frac{\beta}{2}\omega} - e^{-\frac{\beta}{2}\omega}) , \tag{38}$$

and where n_{th} denotes the average number of quanta at temperature T,

$$n_{th} = \frac{1}{e^{\beta\omega} - 1} . \tag{39}$$

Eq. (37) coincides with the Lax–Louisell master equation for the harmonic oscillator in the energy representation and evaluated in the Rotating Wave Approximation (RWA) [18,4]

$$\frac{d\overline{\rho}_S}{dt} = -i\omega[a^\dagger a, \overline{\rho}_S] + \gamma(2a\overline{\rho}_S a^\dagger - a^\dagger a\overline{\rho}_S - \overline{\rho}_S a^\dagger a)$$
$$+ 2\gamma n_{th}(a\overline{\rho}_S a^\dagger + a^\dagger\overline{\rho}_S a - a^\dagger a\overline{\rho}_S - \overline{\rho}_S aa^\dagger) \ . \tag{40}$$

The RWA amounts to neglecting rapidly oscillating terms in the interaction and is valid for weak damping, $\gamma \ll \omega$. The coincidence between our result and the Lax–Louisell master equation does not extend to the time dependence of the non–diagonal elements $\langle n|\overline{\rho}_S|n'\rangle$ with $n \neq n'$ of the reduced density operator. This is due to the form (6) of the second moment which supposes that the entire interaction acts as a random matrix: In our approach, the gain term for these non–diagonal elements vanishes because of the Kronecker delta for the states of the system S appearing in condition (II).

For the harmonic oscillator, Markovian master equations cannot simultaneously fulfill the following three conditions: (i) The reduced density operator is positive definite for all times $t > 0$; (ii) for $t \to \infty$, the reduced density operator attains thermodynamic equilibrium; (iii) in the classical limit, the equation is equivalent to a Langevin equation. This was shown in Ref. [19]. The master equation (40) is of the Lindblad form [20] which guarantees the positivity of the reduced density operator. As a consequence, the quantum–classical correspondence with the Langevin equation is lost, however.

5.2 Case (I)

We first evaluate the generalized transition probabilities of Eq. (32). We proceed in complete analogy to case (II). We find, for instance,

$$W^{(1)}_{nn_1 n_1 n_2} = 2\pi A_0 Q_{nn_1} Q_{n_1 n_2} e^{\frac{\beta}{2}(E_{n_2} - E_{n_1})} e^{-\frac{(E_{n_2} - E_{n_1})^2}{2\Delta^2}} \ . \tag{41}$$

Using the explicit form of the matrix elements Q, we get

$$W^{(1)}_{nn-1n-1n} = W_0 n e^{\frac{\beta\omega}{2}} \qquad W^{(1)}_{nn+1n+1n+2} = W_0\sqrt{(n+1)(n+2)}\ e^{\frac{\beta\omega}{2}}$$
$$W^{(1)}_{nn+1n+1n} = W_0(n+1)e^{-\frac{\beta\omega}{2}} \quad W^{(1)}_{nn-1n-1n-2} = W_0\sqrt{n(n-1)}e^{-\frac{\beta\omega}{2}} \tag{42}$$

where W_0 is given by Eq. (35). Proceeding analogously for the other transition probabilities and inserting the result into the master equation, we obtain

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$$\frac{d}{dt}\langle n|\overline{\rho}_S(t)|n'\rangle = -i\omega(n-n')\langle n|\overline{\rho}_S(t)|n'\rangle)$$

$$-\gamma n_{th}\left(\sqrt{n(n-1)}\langle n-2|\overline{\rho}_S|n'\rangle + (n+1)\langle n|\overline{\rho}_S|n'\rangle\right)$$

$$-\gamma(n_{th}+1)\left(n\langle n|\overline{\rho}_S|n'\rangle + \sqrt{(n+1)(n+2)}\langle n+2|\overline{\rho}_S|n'\rangle\right)$$

$$-\gamma n_{th}\left(\sqrt{n'(n'+1)}\langle n|\overline{\rho}_S|n'-2\rangle + (n'+1)\langle n|\overline{\rho}_S|n'\rangle\right)$$

$$-\gamma(n_{th}+1)\left(n'\langle n|\overline{\rho}_S|n'\rangle + \sqrt{(n'+1)(n'+2)}\langle n|\overline{\rho}_S|n'+2\rangle\right)$$

$$+\gamma n_{th}\left(\sqrt{nn'}\langle n-1|\overline{\rho}_S|n'-1\rangle + \sqrt{n(n'+1)}\langle n-1|\overline{\rho}_S|n'+1\rangle\right)$$

$$+\gamma(n_{th}+1)\left(\sqrt{(n+1)n'}\langle n+1|\overline{\rho}_S|n'-1\rangle\right)$$

$$+\gamma n_{th}\left(\sqrt{nn'}\langle n-1|\overline{\rho}_S|n'-1\rangle + \sqrt{(n+1)n'}\langle n+1|\overline{\rho}_S|n'-1\rangle\right)$$

$$+\gamma(n_{th}+1)\left(\sqrt{n(n'+1)}\langle n-1|\overline{\rho}_S|n'\rangle\right)$$

$$+2\gamma(n_{th}+1)\left(\sqrt{(n+1)(n'+1)}\langle n+1|\overline{\rho}_S|n'+1\rangle\right) \tag{43}$$

It is easy to check that this result coincides with the master equation in energy representation derived (without RWA) by Agarwal for a harmonic oscillator linearly coupled to a bath,

$$\frac{d\overline{\rho}_S}{dt} = -i\omega[a^\dagger a, \overline{\rho}_S]$$
$$- \gamma(a^\dagger a\overline{\rho}_S - 2a\overline{\rho}_S a^\dagger + \overline{\rho}_S a^\dagger a + a^2\overline{\rho}_S - a\overline{\rho}_S a - a^\dagger \overline{\rho}_S a^\dagger + \overline{\rho}_S a^{\dagger 2})$$
$$- \gamma n_{th}\left(2[a^\dagger,[a,\overline{\rho}_S]] + [a^\dagger,[a^\dagger,\overline{\rho}_S]] + [a,[a,\overline{\rho}_S]]\right) . \tag{44}$$

The bath was modeled as an infinite set of harmonic oscillators, and the projection operator technique was used [4].

5.3 Fluctuation–Dissipation Theorem and High–Temperature Limit

With the help of Eq. (35), Eq. (38) for γ takes the form

$$\gamma = \frac{A_0\pi}{M\omega}e^{-\frac{\omega^2}{2\Delta^2}}sinh\frac{\beta}{2}\omega . \tag{45}$$

This equation expresses the fluctuation–dissipation relation. We see that a small band width Δ tends to exponentially decrease the damping coefficient. In view of our *ansatz* for the interaction between system and bath, this fact is not surprising. In the limit of large band width, $\Delta \gg \omega$, Eq. (45) reduces to

the Agarwal fluctuation–dissipation relation [4] between the friction coefficient γ and the diffusion coefficient D,

$$\gamma = \frac{D}{M\omega} e^{\frac{\beta\omega}{2}} sinh\frac{\beta}{2}\omega \ . \tag{46}$$

Here the diffusion constant D is determined by the strength of the coupling,

$$D = A_0 \pi e^{-\frac{\beta\omega}{2}} \ . \tag{47}$$

In the high–temperature limit $\beta\omega \ll 1$, Eq. (46) reduces to the Einstein relation

$$\gamma = \frac{D}{2MkT} \ . \tag{48}$$

We also note that using $a = \left(\sqrt{\frac{M\omega}{2}}x + i\sqrt{\frac{1}{2M\omega}}p\right)$ in Eq. (44) we find the Caldeira–Leggett master equation [6]

$$\frac{d\overline{\rho}_S}{dt} = -i\omega\left[H_S, \overline{\rho}_S\right] - i\gamma\left[x, \{p, \overline{\rho}_S\}\right] - D\left[x, \left[x, \overline{\rho}_S\right]\right] \ . \tag{49}$$

This equation does not have the Lindblad form. This implies that the positivity of the reduced density operator can be violated for certain initial states. In Ref. [21], it was shown that positivity is guaranteed provided the dispersion $\sigma_{xx} =< x^2 > - < x >^2$ of the initial wave packet obeys the condition $\sigma_{xx} \geq \lambda_{dB}^2$.

6 Second Application: Two–level system

We derive the master equation for a two–level system with upper (lower) level $|+\rangle$ $(|-\rangle$, respectively). We introduce the Pauli spin matrices σ_x, σ_y and σ_z. The Hamiltonian of the system takes the form

$$H_S = \frac{1}{2}\omega_0\sigma_z \tag{50}$$

where ω_0 is the energy separation between the two levels. We write $E_n = \frac{1}{2}\omega_0 n$, $n = \pm 1$ and take $Q = \sigma_x$. For the generalized transition probabilies we find

$$W^{(1)}_{+--+} = W_0 e^{\frac{\beta}{2}\omega_0}$$
$$W^{(1)}_{-++-} = W_0 e^{-\frac{\beta}{2}\omega_0} \tag{51}$$

and similar expressions for $W^{(2)}$, $W^{(3)}$ and $W^{(4)}$. Here W_0 is given by Eq. (35) with ω replaced by ω_0 and M set to unity. Thus,

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$$\frac{d}{dt}\langle+|\overline{\rho}_S|+\rangle = -\frac{1}{2}W_0 e^{\frac{\beta}{2}\omega_0}\langle+|\overline{\rho}_S|+\rangle - \frac{1}{2}W_0 e^{\frac{\beta}{2}\omega_0}\langle+|\overline{\rho}_S|+\rangle$$
$$+\frac{1}{2}e^{-\frac{\beta}{2}\omega_0}\langle-|\overline{\rho}_S|-\rangle + \frac{1}{2}e^{-\frac{\beta}{2}\omega_0}\langle-|\overline{\rho}_S|-\rangle$$
$$= -2\gamma(n_{th}+1)\langle+|\overline{\rho}_S|+\rangle + 2\gamma n_{th}\langle-|\overline{\rho}_S|-\rangle \qquad (52)$$

and, in a similar way,

$$\frac{d}{dt}\langle-|\overline{\rho}_S|-\rangle = -2\gamma n_{th}\langle-|\overline{\rho}_S|-\rangle + 2\gamma(n_{th}+1)\langle+|\overline{\rho}_S|+\rangle \ ,$$
$$\frac{d}{dt}\langle-|\overline{\rho}_S|+\rangle = i\omega_0\langle-|\overline{\rho}_S|+\rangle - \gamma(2n_{th}+1)\left[\langle-|\overline{\rho}_S|+\rangle - \langle+|\overline{\rho}_S|-\rangle\right] \ ,$$
$$\frac{d}{dt}\langle+|\overline{\rho}_S|-\rangle = -i\omega_0\langle+|\overline{\rho}_S|-\rangle - \gamma(2n_{th}+1)\left[\langle+|\overline{\rho}_S|-\rangle - \langle-|\overline{\rho}_S|+\rangle\right] \ . \quad (53)$$

Here n_{th} is given by Eq. (39) with ω replaced by ω_0. Simple manipulations with the spin matrices show that the master equation for the two–level system may be written as

$$\frac{d}{dt}\overline{\rho}_S = -2\gamma(n_{th}+1)\,\sigma_+\sigma_-\overline{\rho}_S\sigma_+\sigma_- + 2\gamma n_{th}\,\sigma_+\overline{\rho}_S\sigma_-$$
$$-i\omega_0\,\sigma_+\sigma_-\overline{\rho}_S\sigma_-\sigma_+ - \gamma(2n_{th}+1)\left[\sigma_+\sigma_-\overline{\rho}_S\sigma_-\sigma_+ - \sigma_+\overline{\rho}_S\sigma_+\right]$$
$$+i\omega_0\,\sigma_-\sigma_+\overline{\rho}_S\sigma_+\sigma_- - \gamma(2n_{th}+1)\left[\sigma_-\sigma_+\overline{\rho}_S\sigma_+\sigma_- - \sigma_-\overline{\rho}_S\sigma_-\right]$$
$$-2\gamma n_{th}\,\sigma_-\sigma_+\overline{\rho}_S\sigma_-\sigma_+ + 2\gamma(n_{th}+1)\,\sigma_-\overline{\rho}_S\sigma_+ \qquad (54)$$

or, more simply,

$$\frac{d}{dt}\overline{\rho}_S = -\frac{1}{2}\omega_0[\sigma_z,\overline{\rho}_S] \qquad (55)$$
$$+\gamma n_{th}(2\sigma_+\overline{\rho}_S\sigma_- + \sigma_+\overline{\rho}_S\sigma_+ + \sigma_-\overline{\rho}_S\sigma_- - \overline{\rho}_S\sigma_-\sigma_+ - \sigma_-\sigma_+\overline{\rho}_S)$$
$$+\gamma(n_{th}+1)(\sigma_+\overline{\rho}_S\sigma_+ + \sigma_-\overline{\rho}_S\sigma_- + 2\sigma_-\overline{\rho}_S\sigma_+ - \sigma_+\sigma_-\overline{\rho}_S - \overline{\rho}_S\sigma_+\sigma_-) \ .$$

We have defined the operators $\sigma_- = |-\rangle\langle+|$ and $\sigma_+ = |+\rangle\langle-|$. For $n_{th} = 0$, Eq. (55) reduces to the Agarwal equation for spontaneous emission of a two–level atom [5]. It may seem surprising that Eq. (55) applies for $T = 0$ where the inequality $\Delta \ll T$ is clearly violated and non-Markovian effects are present. In Ref. [22] it was shown that the high–temperature master equation is obeyed even at low temperatures provided the time t is larger than the memory time of the bath, $t \gg t_B$. This implies that condition ii) of Section (3) may be replaced by the less restrictive condition $t_B \ll t \ll t_P$.

7 Conclusion

Starting from a random band–matrix model for the system–bath interaction, we have derived a Markovian master equation for the average reduced density operator of a one–dimensional quantum system. We have assumed that the system–bath interaction is linear in the position coordinate of the quantum system, and we have considered two cases: (I) That part of the interaction which depends on the bath variables is a member of an ensemble of random matrices of proper symmetry; (II) the entire interaction is a member of an ensemble of random matrices of proper symmetry. The form of the master equation differs in both cases. The equation is valid in a domain of parameter values specified by the inequalities i) and ii) of Section 3.

We have applied the master equation to two cases, the damped harmonic oscillator and the dissipative two–level system. For the damped harmonic oscillator and case (I), we have obtained the same equation as Argawal who considered a harmonic oscillator coupled to a heat bath which was modeled as an infinite set of harmonic oscillators. In the limit of high temperature, this equation coincides with the master equation of the Caldeira–Leggett model. For case (II), our master equation for the diagonal elements of the reduced density operator is identical to the Lax–Louisell master equation evaluated in the Rotating Wave Approximation (RWA). This is because in case (II) we impose conditions upon the interaction matrix elements of the position coordinate of the quantum system. These conditions are tantamount to the RWA. For the non–diagonal elements of the reduced density operator, these same conditions imply the vanishing of the gain terms. In this point our result differs from that obtained by Lax and Louisell. For the two–level system and case (I), our master equation reduces, at $T = 0$, to the Argawal equation for spontaneous emission of a two–level atom.

We conclude that Markovian master equations for quantum Brownian motion derived in the weak coupling limit possess universal validity: These equations are independent of the specific microscopic model used for their derivation. This is not true of approximations like the Rotating Wave Approximation. Typically, such approximations violate certain invariance requirements (translational invariance in the case of the RWA) and, thereby, lose universal validity.

A Appendix

The equivalence of Eqs. (10) and (11) is closely related to the equivalence of the microcanonical and the canonical ensemble in the thermodynamic limit $N \rightarrow \infty$ [23]. We thus consider a thermodynamical system in contact with a

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heat bath. The (canonical) partition function is given by

$$Z(\beta) = \int_0^\infty d\varepsilon \rho(\varepsilon) e^{-\beta\varepsilon} = \int_0^\infty d\varepsilon e^{-\beta\varepsilon + \ln \rho(\varepsilon)} \ . \tag{A.1}$$

Since ε and $\ln \rho(\varepsilon)$ grow with N, the integral can be evaluated by a saddle–point approximation. Expanding the integrand up to second order around its maximum ε^*, we get

$$Z(\beta) = \rho(\varepsilon^*) e^{-\beta\varepsilon^*} \int_0^\infty d\varepsilon \ \exp\left(\frac{1}{2}(\varepsilon - \varepsilon^*)^2 \left(\frac{\partial^2 \ln \rho(\varepsilon)}{\partial \varepsilon^2}\right)_{\varepsilon=\varepsilon^*}\right) \ . \tag{A.2}$$

The distribution in energy is a Gaussian centered at ε^* with a width

$$\Delta\varepsilon = \sqrt{-\left(\frac{\partial^2 \ln \rho(\varepsilon)}{\partial \varepsilon^2}\right)} = \sqrt{kT^2 C_V} \ . \tag{A.3}$$

We have used the fact that $k \ln \rho(\varepsilon)$ is the microcanonical entropy. For $N \to \infty$, $\Delta\varepsilon/\varepsilon^* \sim 1/\sqrt{N}$ becomes negligibly small and the Gaussian approaches a δ-function. Hence,

$$\hat{\rho}_B(0) = \frac{1}{Z} \sum_a e^{-\beta\varepsilon_a} |a\rangle\langle a| \simeq |a^*\rangle\langle a^*| \tag{A.4}$$

where $|a^*\rangle$ is the eigenvector corresponding to the eigenvalue ε^*. Moreover, according to Eq. (A.2) the density of states can be approximated locally by

$$\rho(\varepsilon^*) = \rho_0 e^{\beta\varepsilon^*} \ . \tag{A.5}$$

B   Appendix

B.1   The average propagator

The propagator $K(t)$ is defined by

$$K(t) = U(t)\theta(t) = e^{-iHt}\theta(t) \tag{B.1}$$

and obeys Dyson's equation

$$K(t) = K_0(t) - i \int_{-\infty}^\infty dt_1 K_0(t - t_1) W K(t_1) \tag{B.2}$$

where $K_0(t) = e^{-iH_0 t}\theta(t)$ is the free propagator and $\theta(t)$ the unit step function.

To calculate the average of $K(t)$, we use the energy representation and introduce the following pair of Fourier transforms

$$G(E) = \frac{1}{i} \int_{-\infty}^{\infty} dt e^{iEt} K(t) \, , \qquad K(t) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} dt e^{-iEt} G(E) \, . \qquad (B.3)$$

The transforms of (B.1) and (B.2) are then given by

$$G(E) = \frac{1}{E - H + i\varepsilon} \qquad \varepsilon \to 0^+ \qquad (B.4)$$

and

$$G = G_0 + G_0 W G = \sum_{s=0}^{\infty} G_0 (W G_0)^s \, , \qquad (B.5)$$

respectively.

To average G, we use Eqs. (5,6) and the rule that the average over a product of Gaussian distributed W's equals the sum over all ways of Wick–contracting pairs of W's. We show below that in the limit of weak coupling, only contractions between adjacent pairs of W's have to be taken into account. We find

$$\overline{G} = \sum_{s=0}^{\infty} \overline{G_0 (W G_0)^s} = G_0 + G_0 \overline{W G_0 W} G_0 + G_0 \overline{W G_0 W} G_0 \overline{W G_0 W} G_0 + \cdots$$

$$= G_0 \frac{1}{1 - \overline{W G_0 W} G_0} \, . \qquad (B.6)$$

B.1.1   Case (II)

Since

$$\langle nb | G_0(E) | n'b' \rangle = \delta_{nn'} \delta_{bb'} \frac{1}{E - (E_n + \varepsilon_b) + i\varepsilon} = \delta_{nn'} \delta_{bb'} (G_0)_{nb} \qquad (B.7)$$

and

$$\langle nb | \overline{W G_0 W} | n'b' \rangle = \sum_{n_1 b_1} \overline{W_{bb_1}^{nn_1} (G_0)_{n_1 b_1} W_{b_1 b'}^{n_1 n'}} (G_0)_{n'b'}$$

$$= \delta_{nn'} \delta_{bb'} (G_0)_{nb} \sum_{n_1 b_1} \overline{W_{bb_1}^{nn_1 2}} (G_0)_{n_1 b_1} \, , \qquad (B.8)$$

the matrix elements of $\overline{G}$ become

$$\langle nb|\overline{G}|n'b'\rangle = \frac{\delta_{nn'}\delta_{bb'}}{E - (E_n + \varepsilon_b) - \sum_{n_1 b_1} \overline{W_{bb_1}^{nn_1 2}}(G_0)_{n_1 b_1}}$$

$$= \frac{\delta_{nn'}\delta_{bb'}}{E - (E_n + \varepsilon_b) - R_{nb}(E)} \tag{B.9}$$

which shows that $\overline{G}$ is diagonal in the unperturbed energy basis. Here,

$$R_{nb}(E) = \Delta_{nb}(E) - i\frac{\Gamma_{nb}(E)}{2} \tag{B.10}$$

where

$$\Delta_{nb}(E) = P \sum_{n_1 b_1} \frac{\overline{W_{bb_1}^{nn_1 2}}}{E - (E_{n_1} + \varepsilon_{b_1})} \ ,$$

$$\Gamma_{nb}(E) = 2\pi \sum_{n_1 b_1} \overline{W_{bb_1}^{nn_1 2}}\delta(E - (E_{n_1} + \varepsilon_{b_1})) \ . \tag{B.11}$$

For sufficiently high temperature, $\Gamma_{nb}(E)$ depends slowly on energy and can be approximated by

$$\Gamma_{nb}(E) \simeq \Gamma_{nb}(E_n + \varepsilon_b) = \Gamma_{nb}$$

$$= 2\pi \sum_{n_1 b_1} \overline{W_{bb_1}^{nn_1 2}}\delta(E_n + \varepsilon_b - E_{n_1} - \varepsilon_{b_1}) \ . \tag{B.12}$$

For the averaged propagator, this yields

$$\overline{G}_{nb}(E) = \frac{1}{E - (E_n + \varepsilon_b) + i\frac{\Gamma_{nb}}{2}} \tag{B.13}$$

where we have neglected the level shift Δ_{nb}. Transforming back to time representation, we obtain

$$\overline{K}_{nb}(t) = e^{-i(E_n t + \varepsilon_b) - \frac{\Gamma_{nb}}{2}t}\theta(t) \ . \tag{B.14}$$

In the limit of weak coupling, contractions between non–adjacent pairs of W's are negligible. This can be shown by inspecting the contributions from the various products of Wick contractions. We consider here the simplest case and compare [24] the imaginary parts of $\langle nb| \ WG_0W \ |n'b'\rangle$ and $\langle nb| \ WG_0WG_0WG_0W \ |n'b'\rangle$ (the real parts represent level shifts and do not contribute to the decay width). We are thus led to compare $\Gamma_{nb}(E)$ with $\sum_{n_1 b_1} \overline{W_{bb_1}^{nn_1 2}}(G_0)_{n_1 b_1}^2 \Gamma_{n_1 b_1}(E)$. These quantities are calculated as in Section 5. Assuming that $|Q_{nn_1}|^2$ vanishes unless the states n_1 and n are close in energy, we find that in the high–temperature limit $\omega \ll \Delta \ll kT$, $\Gamma_{nb}(E)$ may be replaced by $\Gamma_{nb}(E_n + \varepsilon_b)$, and that in the weak–coupling limit $\gamma \ll \Delta$, the second term may be omitted in comparison with the first.

B.1.2 Case(I)

In this case, the propagator is not diagonal in the energy representation and we have instead

$$\langle nb|\overline{G}|n'b'\rangle = \delta_{bb'}\langle nb|\overline{G}|n'b\rangle . \tag{B.15}$$

As a consequence, the series (B.6) is not geometric any more and cannot be summed easily. We thus have to find another method to evaluate the average propagator. We actually calculate only the time derivative of the average propagator which is sufficient for the derivation of the master equation.

Iterating the Dyson equation (B.5) once

$$G = G_0 + G_0W + G_0WG_0WG \tag{B.16}$$

and taking the average

$$\overline{G} = G_0 + G_0\overline{W} + G_0\overline{WG_0WG} = G_0 + G_0\overline{WG_0W}\,\overline{G} \tag{B.17}$$

yields the same result as in Eq. (B.6). We use this fact to average the time–evolution operator. In the interaction picture, we have

$$i\frac{d\tilde{U}(t)}{dt} = \tilde{W}(t)\tilde{U}(t) \qquad\qquad \tilde{U}(0) = U(0) = 1 \tag{B.18}$$

where

$$\tilde{U}(t) = e^{iH_0 t}U(t) \qquad \text{and} \qquad \tilde{W}(t) = e^{iH_0 t}We^{-iH_0 t} . \tag{B.19}$$

This equation can also be written in integral form

$$\tilde{U}(t) = 1 - i\int_0^t dt_1 \tilde{W}(t_1)\tilde{U}(t_1) . \tag{B.20}$$

Inserting Eq. (B.20) into Eq. (B.18) and averaging, we find

$$\frac{\overline{d\langle nb|\tilde{U}(t)|nb\rangle}}{dt} =$$

$$-\int_0^t dt_1 \sum_{\substack{n_1 b_1 \\ n_2 b_2}} \overline{\langle nb|\tilde{W}(t)|n_1 b_1\rangle\langle n_1 b_1|\tilde{W}(t_1)|n_2 b_2\rangle}\,\overline{\langle n_2 b_2|\tilde{U}(t_1)|nb\rangle} . \tag{B.21}$$

We have $\overline{W_{bb_1}^{nn_1}W_{b_1 b_2}^{n_1 n_2}} = \delta_{bb_2}Q_{nn_1}Q_{n_1 n_2}\overline{V_{bb_1}}^2$, hence

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$$\frac{d\overline{\langle nb|\tilde{U}(t)|n'b\rangle}}{dt} = -\int_0^t d\tau \sum_{n_1 b_1 n_2} e^{i(E_n - E_{n_2})t} e^{i(E_{n_2} + \varepsilon_b - E_{n_1} - \varepsilon_{b_1})\tau}$$
$$\times Q_{nn_1} Q_{n_1 n_2} \overline{V_{bb_1}}^2 \, \overline{\langle n_2 b|\tilde{U}(t-\tau)|n'b\rangle} \tag{B.22}$$

where we have set $\tau = t - t_1$. In the weak–coupling limit $d\overline{\tilde{U}}/dt$ is small and $\overline{\tilde{U}(t-\tau)}$ may be replaced by $\overline{\tilde{U}(t)}$. This approximation amounts to neglecting memory effects and is thus a Markov approximation. We obtain,

$$\frac{d\overline{\langle nb|\tilde{U}(t)|n'b\rangle}}{dt} = -\frac{1}{2} \sum_{n_1 n_2} W^{(1)}_{nn_1 n_1 n_2} e^{i(E_n - E_{n_2})t} \, \overline{\langle n_2 b|\tilde{U}(t)|n'b\rangle} \ . \tag{B.23}$$

We have defined

$$W^{(1)}_{nn_1 n_1 n_2} = 2\pi \sum_{b_1} Q_{nn_1} Q_{n_1 n_2} \overline{V_{bb_1}}^2 \delta(E_{n_2} + \varepsilon_b - E_{n_1} - \varepsilon_{b_1}) \ . \tag{B.24}$$

In the Schrödinger picture,

$$\frac{d\overline{\langle nb|U(t)|n'b\rangle}}{dt} = -i(E_n + \varepsilon_b)\overline{\langle nb|U(t)|n'b\rangle}$$
$$-\frac{1}{2} \sum_{n_1 n_2} W^{(1)}_{nn_1 n_1 n_2} \, \overline{\langle n_2 b|U(t)|n'b\rangle} \ . \tag{B.25}$$

We have similarly

$$\frac{d\overline{\langle nb|U^\dagger(t)|n'b\rangle}}{dt} = i(E_{n'} + \varepsilon_b)\overline{\langle nb|U^\dagger(t)|n'b\rangle}$$
$$-\frac{1}{2} \sum_{n_1 n_2} W^{(2)}_{n_2 n_1 n_1 n'} \, \overline{\langle nb|U^\dagger(t)|n_2 b\rangle} \tag{B.26}$$

with

$$W^{(2)}_{n_1 n' n_2 n_1} = 2\pi \sum_{b_1} Q_{n_1 n'} Q_{n_2 n_1} \overline{V_{bb_1}}^2 \delta(E_{n_2} + \varepsilon_b - E_{n_1} - \varepsilon_{b_1}) \ . \tag{B.27}$$

B.2 The evolution equation for the average density operator

The general density operator at times t, t' is given by

$$\hat{\rho}(t, t')\theta(t)\theta(t') = K(t)\hat{\rho}(0)K^\dagger(t') \tag{B.28}$$

where we have used the definition (A.2) for the propagator. We take the double Fourier transform and obtain

$$\hat{\rho}(E, E') = G(E)\hat{\rho}(0)G^{\dagger}(E') \tag{B.29}$$

where $G(E)$ is given by Eq. (B.5). Hence

$$\overline{\rho}(E, E') = \sum_{s=0}^{\infty}\sum_{r=0}^{\infty} \overline{G_0(WG_0)^s\hat{\rho}(0)(G_0^{\dagger}W)^rG_0^{\dagger}} \ . \tag{B.30}$$

In the weak–coupling limit, $\overline{G}$ appears sandwiched between two W's which are contracted across $\hat{\rho}(0)$, and the general term in the expansion (B.30) attains the form

$$\overline{G}\overline{W\cdots W\overline{G}\hat{\rho}(0)\overline{G}^{\dagger}W\cdots W}\overline{G}^{\dagger} \ . \tag{B.31}$$

Thus,

$$\overline{\rho} = \overline{G}\hat{\rho}(0)\overline{G}^{\dagger} + \overline{G}\overline{W\overline{G}\hat{\rho}(0)\overline{G}^{\dagger}W}\overline{G}^{\dagger}$$
$$+ \overline{G}\overline{W\overline{G}\ \overline{W\overline{G}\hat{\rho}(0)\overline{G}^{\dagger}W}\overline{G}^{\dagger}W}\overline{G}^{\dagger} + \cdots \tag{B.32}$$

or

$$\overline{\rho} = \overline{G}\hat{\rho}(0)\overline{G}^{\dagger} + \overline{G}\overline{W\overline{G}\overline{\rho}\,\overline{G}^{\dagger}W}\overline{G}^{\dagger} \ . \tag{B.33}$$

Eq. (B.33), together with Eq. (B.6) for $\overline{G}$, completely determines the dynamics of the system. Transforming back to the time representation, we can rewrite these equations as

$$\overline{\rho}(t, t')\theta(t)\theta(t') = \overline{K}(t)\hat{\rho}(0)\overline{K}^{\dagger}(t')$$
$$+ \int\limits_{-\infty}^{\infty} d\tau \int\limits_{-\infty}^{\infty} d\tau'\overline{K}(t-\tau)\overline{W\,\overline{\rho}(\tau, \tau')\theta(\tau)\theta(\tau')W}\overline{K}^{\dagger}(t'-\tau') \quad \text{(B.34)}$$

and

$$\overline{K}(t) = K_0(t) + \int\limits_{-\infty}^{\infty} dt_1 \int\limits_{-\infty}^{\infty} dt_2 K_0(t-t_1)\overline{W\,K_0(t_1-t_2)\,W}\,\overline{K}(t_2) \ . \quad \text{(B.35)}$$

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