Non-Markovian modeling of Fermi-Bose systems coupled to one or several Fermi-Bose thermal baths

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(Received 15 April 2020; accepted 23 July 2020; published 11 August 2020)

A method is proposed to describe Fermi or Bose systems coupled to one or several heat baths composed of fermions and/or bosons. The method, called the coupled equations of motion method, properly includes non-Markovian effects. The approach is exact in the full-coupling approximation when only bosonic particles are present in the system and baths. The approach provides an approximate treatment when fermions are present either in the system and/or in one or several environments. Our approach has the advantage of properly respecting the Pauli exclusion principle for fermions during the evolution. We illustrate the approach for the single fermionic or bosonic oscillator coupled to one or two heat baths assuming different types of quantum statistics (fermion or boson) for them. The cases of a Fermi system coupled to fermion or boson heat baths or a mixture of both are analyzed in detail. With the future goal of treating Fermi systems formed of an increasing number of two-level systems (qubits), we discuss possible simplifications that could be made in the equations of motion and their limits of validity in terms of the system-bath coupling or of the initial heat bath temperatures.

DOI: [10.1103/PhysRevA.102.022209](https://doi.org/10.1103/PhysRevA.102.022209)

I. INTRODUCTION

The description of dissipation and decoherence is an important subject of investigation, especially in view of the current boom in quantum technologies [\[1,2\]](#page-10-0) (see also the discussion in Ref. [\[3\]](#page-10-0)). In this field, the system of interest is a number of qubits that are inherently coupled to one or several environments [\[4–6\]](#page-10-0). The effect of this coupling is rather dramatic since it induces a nonunitary evolution of the system, and ultimately tends to destroy the interesting quantum aspects, driving the system to classical physics. Controlling the transition from quantum to classical physics is becoming crucial in this context. By changing the properties of the baths, one might first study the transition from the Markovian to the non-Markovian regime. In particular, it has been recently underlined that non-Markovian dynamics and their impact should be explored more systematically [\[1,2\]](#page-10-0).

Non-Markovian effects and their description is an active field of research in the theory of open quantum systems [\[7–10\]](#page-10-0), especially with the aim of developing accurate and versatile approaches. With the progress of manipulating atoms and molecules, one might engineer systems and/or environments that can be formed of fermionic or bosonic particles. Another example is the atomic nuclei where nucleons (fermions) act as a reservoir for the collective excitations treated as bosons [\[11\]](#page-10-0). Treating fermions is finally of special interest in the context of quantum computing due to the oneto-one mapping between spin systems and fermions on lattices [\[12\]](#page-11-0).

Our primary goal here is to develop a unified approach able to describe fermions or bosons coupled to a set of baths that can also be a mixture of fermions and bosons. Systems coupled to several reservoirs are of special interest in different fields of physics. To quote a few of them, we mention the example of cavity quantum electrodynamics [\[13\]](#page-11-0), Jaynes-Cummings lattices [\[14\]](#page-11-0), photon-ion interfaces [\[15\]](#page-11-0), ion chain systems [\[16\]](#page-11-0), or phonon-induced spin squeezing [\[17\]](#page-11-0) (see also examples in Refs. [\[18–21\]](#page-11-0)).

In the following, we first recall some recent progress we have made in the description of systems coupled to several heat baths $[21-27]$. We then discuss in detail the extra subtleties that appear for Fermi systems or environments compared to the Bose case. In the case of the bosonic system and environments, an exact treatment is *a priori* possible including fully the non-Markovian effects. When fermions are present in the system or in the surrounding baths, some approximations are required. We describe in Sec. [III](#page-3-0) a specific methodology to treat a Fermi system coupled to Fermi, Bose, or Fermi-Bose mixtures of baths. In this approach, where the non-Markovian effects are included, special attention is paid to respect the Pauli exclusion principle for Fermi degrees of freedom. The approach is then illustrated for the system coupled to one or several heat baths in Sec. [IV.](#page-5-0)

II. METHOD

We follow here our previous work $[21-27]$ and consider a Fermi or Bose system coupled to one or several baths. Some of the baths could be composed of fermions and some other of bosons. In our previous studies we gradually considered

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problems of increasing complexity, i.e., changing the quantum statistics of the system or bath, considering more general coupling, and/or increasing the number of baths.

A single fermionic or bosonic oscillator coupled to an environment is considered. The system+environment Hamiltonian is taken as

$$
H = HS + HE + HSE.
$$
 (1)

The system and environment Hamiltonians, denoted respectively by H_S and H_E , are given by

$$
H_{\rm S} = \hbar \omega_1 a_1^{\dagger} a_1, \quad H_{\rm E} = \sum_{\nu} \hbar \omega_{\nu} a_{\nu}^{\dagger} a_{\nu}.
$$
 (2)

For the moment, we do not specify if there is one or several baths and simply assume that the quantum nature (fermionic or bosonic) of each pair of creation or annihilation operators $(a_{\nu}^{\dagger}, a_{\nu})$ is specified through the relation

$$
a_{\nu}a_{\nu}^{\dagger} = 1 + \varepsilon_{\nu}a_{\nu}^{\dagger}a_{\nu}, \qquad (3)
$$

where $\varepsilon_v = +1$ (−1) for bosons (fermions). We also use the convention $v = 1$ ($v > 1$) for the system (for the environment). Note that, in the present model, the fermionic heat bath is described by an infinite set of two-level systems initially at thermal equilibrium. Besides the commutation or anticommutation rules of creation or annihilation operators, the difference between a bosonic and fermionic bath stems from the initial occupation probability denoted by $n(\omega_v)$ that corresponds either to Bose-Einstein or Fermi-Dirac occupation probability. A pictorial view of the heat bath was given in Fig. 1 of Ref. [\[23\]](#page-11-0).

In the following, we will consider the full-coupling case (FC), in which the coupling between the system and environ-

FIG. 1. Time evolution of the occupation probability in the system $n_1(t) = M_{11}(t)$ obtained by solving Eqs. [\(8\)](#page-2-0) (red solid line) or by solving the set of equations (16) (black dashed line). Panels (a) and (c) correspond to the case of a bosonic system coupled to a bosonic bath starting from $n_1(0) = 0$ and $n_1(1) = 1$, respectively. Panels (b) and (d) correspond to the case of a fermionic system coupled to a fermionic bath again starting from $n_1(0) = 0$ and $n_1(1) = 1$, respectively. In all cases, the bath properties are given by $c_1 = 0.1$, $\gamma_1/\Omega = 12$, and $T_1/\Omega = 1$. Note that, in the B-B case, the two approaches are equivalent and the two curves displayed in panels (a) and (c) cannot be distinguished.

ment is as follows:

$$
H_{\rm SE} = H_{\rm FC} = \sum_{\nu > 1} g_{\nu} (a_1^{\dagger} + a_1) (a_{\nu}^{\dagger} + a_{\nu}). \tag{4}
$$

The present formulation is rather flexible and includes the possibility that some environmental particles obey fermion statistics while others obey boson statistics. It also includes the possibility that the environment can be decomposed into several baths with eventually different quantum natures and different initial temperatures. We note that the Hamiltonian (1) can be used to describe a single qubit surrounded by one or several heat baths. In our previous work, we used the Heisenberg representation to obtain a solution to the system+environment problem taking into account possible non-Markovian effects [\[21–27\]](#page-11-0). The solution we provided, once the frequency is properly renormalized (see discussion below), is exact for the FC coupling when only bosonic particles are considered for both the system and the heat baths. The situation is more delicate in the FC case when fermions (either in the bath and/or one of the environments) are involved. In this case, the problem could not be solved exactly and a specific prescription should be made to obtain a closed form of the equations of motion to be solved. A first solution to this problem was given in Refs. [\[22,25\]](#page-11-0). Such a solution resulted in a quite reasonable description of the Fermi systems coupled to one or several baths. Numerical applications have recently shown however that occupation numbers of the systems with the fermionic heat bath(s) can sometimes slightly exceed 1. This points out that some modifications of the method might be needed. Another interesting result was the absence of an asymptotic stationary solution when the system is coupled to a mixture of fermionic and bosonic heat baths [\[26\]](#page-11-0). In the following, we propose an alternative solution that avoids the occurrence of nonphysical occupation numbers during the evolution.

A. Summary and illustration of our previous work

We summarize here the strategy we employed previously starting from the Heisenberg equations of motion for the system and heat-bath creation operators:

$$
\frac{d}{dt}a_1^{\dagger} = i\omega_1 a_1^{\dagger} + i(1 - [1 - \varepsilon_1]a_1^{\dagger} a_1) \sum_{v} g_v [a_v^{\dagger} + a_v], \quad (5)
$$

$$
\frac{d}{dt}a_{\alpha}^{\dagger} = i\omega_{\alpha}a_{\alpha}^{\dagger} + ig_{\alpha}(1 - [1 - \varepsilon_{\alpha}]a_{\alpha}^{\dagger}a_{\alpha})[a_{1}^{\dagger} + a_{1}].
$$
 (6)

When all particles are bosons, we have $[1 - \varepsilon_1] = [1 - \varepsilon_\alpha] =$ 0 for all $\alpha > 1$. The equations of motion become a linear set of equations between the creation and annihilation operators. In this case, the problem is solved exactly using the Laplace transform technique (see, for instance, Ref. [\[23\]](#page-11-0)). In Refs. [\[24,25\]](#page-11-0), we have also illustrated that such a problem can be accurately solved by using the discretized environment method (DEM) together with the special Bogolyubov transformation [\[28\]](#page-11-0) between the creation and annihilation operators (see Sec. [IV](#page-5-0) of Ref. [\[25\]](#page-11-0)). An alternative solution to the present problem could be to consider directly the coupled equations of motion (CEM) for the normal and anomalous densities, denoted respectively by *M* and *K*, associated to the

system+environment. Using the notations¹

$$
M_{\nu\alpha} = \langle a_{\nu}^{\dagger} a_{\mu} \rangle, \quad G_{\nu\alpha}(t) = \langle a_{\nu} a_{\alpha}^{\dagger} \rangle,
$$

$$
K_{\nu\alpha} = \langle a_{\nu}^{\dagger} a_{\alpha}^{\dagger} \rangle, \quad K_{\nu\alpha}^{*} = \langle a_{\alpha} a_{\nu} \rangle,
$$
 (7)

we obtain for the boson system coupled to the bosonic environment the set of coupled equations for the *M* and *K* components:

$$
\frac{dM_{11}}{dt} = i \sum_{\nu} g_{\nu} (M_{\nu 1} - M_{1\nu}) + i \sum_{\nu} g_{\nu} (K_{1\nu}^{*} - K_{1\nu}),
$$
\n
$$
\frac{dM_{1\alpha}}{dt} = i(\omega_{1} - \omega_{\alpha}) M_{1\alpha} + i \sum_{\nu} g_{\nu} (M_{\nu\alpha} + K_{\alpha\nu}^{*}) - ig_{\alpha} (M_{11} + K_{11}),
$$
\n
$$
\frac{dM_{\alpha\beta}}{dt} = i(\omega_{\alpha} - \omega_{\beta}) M_{\alpha\beta} + ig_{\alpha} (M_{1\beta} + K_{\beta 1}^{*}) - ig_{\beta} (M_{\alpha 1} + K_{\alpha 1}),
$$
\n
$$
\frac{dK_{11}}{dt} = 2i\omega_{1} K_{11} + i \sum_{\nu} g_{\nu} (K_{\nu 1} + M_{1\nu} + G_{\nu 1} + K_{1\nu}),
$$
\n
$$
\frac{dK_{1\alpha}}{dt} = i(\omega_{1} + \omega_{\alpha}) K_{1\alpha} + i \sum_{\nu} g_{\nu} (G_{\nu\alpha} + K_{\nu\alpha}) + ig_{\alpha} (M_{11} + K_{11}),
$$
\n
$$
\frac{dK_{\alpha\beta}}{dt} = i(\omega_{\alpha} + \omega_{\beta}) K_{\alpha\beta} + ig_{\alpha} (G_{1\beta} + K_{1\beta}) + ig_{\beta} (M_{\alpha 1} + K_{\alpha 1}).
$$
\n(8)

Solving these equations numerically, we obtain the exact solution of the problem when only bosons are presented in both the system and baths. As illustrated below, this method is strictly equivalent to the one we used in Refs. [\[23,24\]](#page-11-0).

B. Numerical solution of Eq. (8) with discretization of heat bath

Here, we consider the system with frequency Ω (we use the convention $\hbar = 1$ throughout the paper) and all energies and coupling constants are given in units of Ω . Time is given in Ω^{-1} units. We assume that the system is coupled to one or several baths. Each bath, labeled by *i*, has a Lorentz-Drude spectral function given by

$$
J_i(\omega) = \frac{c_i}{\pi} \omega \frac{\gamma_i^2}{\gamma_i^2 + \omega^2}.
$$
 (9)

The two parameters c_i and γ_i determine the coupling strength with the system and the memory effect, respectively. In order to solve the CEM, a finite discrete number of levels ν is used for each environment. In practice, we follow the procedure proposed in Ref. [\[24\]](#page-11-0). For a given environment, a finite set of frequencies ω_{ν} is used according to

$$
\omega_{\nu} = \Delta \omega (n + 1/2), \quad n = 0, \dots, N_{\text{max}}.
$$
 (10)

Then, the coupling g_{ν} entering in the Hamiltonian is given by $g_v = \sqrt{\Delta \omega J_i(\omega_v)}$. Further details and discussions can be found in Ref. [\[24\]](#page-11-0). Note that the discretization of ω can be taken nonuniform. In practice, small $\Delta\omega$ are required only in the vicinity of Ω to get a good numerical accuracy and larger $\Delta\omega$ can be used away from the system frequency. We use this property to reduce the total number of states necessary

for each bath. In the following applications, we use $N_{\text{max}} =$ 400 states with $\Delta\omega$ that depends on *n* such that $\Delta\omega_{n+1} =$ $\lambda \Delta \omega_n$ with $\Delta \omega_0 / \Omega = 0.01$ and $\lambda = 1.015$. The choice of the values for three parameters $\Delta\omega_0$, λ , and N_{max} is critical to properly achieve good numerical accuracy. In particular, these parameters should be chosen in such a way that $\Delta \omega_n \ll \Omega$ in the vicinity of Ω and $T \ll \omega_{N_{\text{max}}}$, while keeping N_{max} not too high in order to obtain the result in a reasonable numerical time. The choice of the parameters for the discretization has been validated for the boson system coupled to a bosonic bath by comparing with the results obtained using the Laplace transform technique [\[23\]](#page-11-0).

To avoid the unphysical shift of the system frequency induced by the coupling with the baths, this frequency is renormalized prior to the calculation as it is always done [\[29\]](#page-11-0). For the FC case, the frequency ω_1 used in Eqs. (8) is as follows:

$$
\omega_1 = \Omega + 4 \sum_{\nu} \frac{g_{\nu}^2}{\omega_{\nu}}.
$$
 (11)

Finally, each heat bath is characterized by its initial temperature T_i such that the initial occupation $n_v(0)$ of the state in the bath *i* is given by (using the convention $k_B = 1$ for the Bolztmann constant)

$$
n_{\nu}(0) = M_{\nu\nu}(0) = \frac{1}{\exp(\omega_{\nu}/T_i) - \varepsilon_{\nu}}.
$$
 (12)

The results are shown in Fig. [1](#page-1-0) for the Bose system coupled to a single bosonic bath. The time evolution of occupation probability is obtained by solving the set of equations (8) for the FC coupling using the discretization of the environment. The results perfectly match those obtained in Ref. [\[23\]](#page-11-0) using the Laplace transform technique. When we write down the creation and annihilation operators a_1^{\dagger} and a_1 (a_v^{\dagger} and a_v), we mean the creation and annihilation operators of transition with the corresponding energy $\hbar \omega_1$ ($\hbar \omega_2$). So, each a_1 (a_{ν}^{\dagger}) and a_1

¹Note that for the sake of simplicity, we use slightly different convention for the indices ordering compared to the standard definition of the normal and anomalous densities in many-body systems [\[11\]](#page-10-0).

 (a_v) is the product of creation and annihilation operators of a particle. In our formalism, there is a conversion of excitation quanta from the fermionic or bosonic system to the bosonic or fermionic environment or vice versa. Since only the level associated to a_1^{\dagger} is populated or depopulated by the coupling, the number of particles in the system as a function of time directly identifies with the quantity $n_1(t)$.

C. Direct extension of Eqs. [\(8\)](#page-2-0) when fermions are involved

In the following, we will systematically use the shorthand notation B-B, F-F, B-F, and F-B, where the first letter refers to the system statistics $(B=$ bosons and $F=$ fermions), while the second letter refers to the bath statistics. When more than one bath is considered, we use the convention System- $Bath_1-Bath_2-\cdots$.

Equations [\(8\)](#page-2-0) provide an exact treatment of the B-B case. Based on simple arguments, we previously proposed to treat the F-F case by neglecting the terms $(1 - \varepsilon_1) \hat{a}_1^{\dagger} a_1$ and $(1 - \varepsilon_1) a_1^{\dagger} a_2$ ε_{α}) $a_{\alpha}^{\dagger} a_{\alpha}$ in Eqs. [\(5\)](#page-1-0) and [\(6\)](#page-1-0) when the system and baths are both composed of fermions. This direct mapping from bosons to fermions has the great advantage to give linear Heisenberg equations also for the F-F case while the bath properly imposes asymptotically the Fermi statistics to the system in the weak-coupling–high-temperature limit. The results of this approximate treatment are also shown in Fig. [1](#page-1-0) for the F-F case. We clearly see in this figure [panel (d)] that, while the asymptotic behavior is expected to be properly treated, the price to pay with the simplified treatment is the occurrence of unphysical behavior at the initial timescale with occupation numbers larger than 1. This stems from the fact that the Pauli exclusion principle might be broken during the time evolution. Indeed, in Eqs. [\(8\)](#page-2-0), nothing prevents one from having $K_{11}(t) = \langle (a_1^{\dagger})^2 \rangle$ nonzero during the evolution even if the system is fermionic.

Nevertheless, the simplified treatment has additional interesting properties that have been used to overcome this difficulty. One of them is the possibility to map exactly Eqs. [\(9\)](#page-2-0) into the simple time-local diffusion equation for the occupation probability:

$$
\frac{dn_1(t)}{dt} = -2\lambda_1(t)n_1(t) + 2D_1(t),\tag{13}
$$

including fully non-Markovian effects. Using this equation and some symmetry properties of the master equation obtained for $n_1(t)$ with the nonlinear termed, it was shown in Ref. [\[22\]](#page-11-0) that the F-B and B-F case can be accurately

FIG. 2. Same as in Fig. [1,](#page-1-0) but for the mixed quantum statistics case of the boson system coupled to the fermion bath (B-F) [(a) and (c)] and for the fermion system coupled to boson bath (F-B) [(b) and (d)]. The bath properties are given by $c_1 = 0.1$, $\gamma_1/\Omega = 12$, and $T_1/\Omega = 1$. In all cases, the red solid line corresponds to the result obtained with the Laplace transform approach in Ref. [\[22\]](#page-11-0). The black dashed line corresponds to the result obtained with Eqs. [\(16\)](#page-4-0).

described using the diffusion equation (13) with modified transport coefficients. This approach leads to the proper asymptotic limit even though the Fermi nature of the system or bath might be slightly broken. The results obtained with this method for the F-B and B-F cases are illustrated in Fig. 2.

III. TREATMENT OF F-F, B-F, AND F-B CASES ENFORCING THE PAULI EXCLUSION PRINCIPLE

In the present paper we propose a treatment that respects the Fermi nature of the particle all along the nonequilibrium evolution. This implies to explicitly account for the nonlinear term in the Heisenberg equation of motion. The situation is similar to the many-body problem of interacting particles where the one-body density-matrix evolution depends on the two-body density, whose evolution is itself coupled to the three-body density and so on and so forth, leading to the so-called Bogolyubov-Born-Green-Kirkwood-Yvon hierarchy [\[30–36\]](#page-11-0).

The general form of the equations of motion, which is valid regardless of the quantum natures of the system or bath, is given as

$$
\frac{d\langle a_1^{\dagger}a_1\rangle}{dt} = i \sum_{v} g_v(\langle a_v^{\dagger}a_1\rangle - \langle a_1^{\dagger}a_v\rangle) + i \sum_{v} g_v(\langle a_v a_1\rangle - \langle a_1^{\dagger}a_v^{\dagger}\rangle),
$$
\n
$$
\frac{d\langle a_1^{\dagger}a_{\alpha}\rangle}{dt} = i(\omega_1 - \omega_{\alpha})\langle a_1^{\dagger}a_{\alpha}\rangle + i \sum_{v} g_v((1 - [1 - \varepsilon_1]a_1^{\dagger}a_1)[a_v^{\dagger}a_{\alpha} + a_v a_{\alpha}]) - ig_{\alpha}\langle (1 - [1 - \varepsilon_{\alpha}]a_{\alpha}^{\dagger}a_{\alpha})[a_1^{\dagger}a_1 + a_1^{\dagger}a_1^{\dagger}]),
$$
\n
$$
\frac{d\langle a_\alpha^{\dagger}a_{\beta}\rangle}{dt} = i(\omega_{\alpha} - \omega_{\beta})\langle a_\alpha^{\dagger}a_{\beta}\rangle + ig_{\alpha}\langle (1 - [1 - \varepsilon_{\alpha}]a_{\alpha}^{\dagger}a_{\alpha})[a_1^{\dagger}a_{\beta} + a_1a_{\beta}]\rangle - ig_{\beta}\langle [a_\alpha^{\dagger}a_1^{\dagger} + a_\alpha^{\dagger}a_1](1 - [1 - \varepsilon_{\beta}]a_{\beta}^{\dagger}a_{\beta})\rangle,
$$
\n
$$
\frac{d\langle a_1^{\dagger}a_1^{\dagger}\rangle}{dt} = 2i\omega_1\langle a_1^{\dagger}a_1^{\dagger}\rangle + i\frac{1 + \varepsilon_1}{2} \sum_{v} g_v(\langle (1 - [1 - \varepsilon_1]a_1^{\dagger}a_1)[a_v^{\dagger}a_1^{\dagger} + a_v a_1^{\dagger}]\rangle + \langle [a_1^{\dagger}a_1^{\dagger} + a_1^{\dagger}a_v](1 - [1 - \varepsilon_1]a_1^{\dagger}a_1)\rangle),
$$

$$
\frac{d\langle a_1^{\dagger}a_\alpha^{\dagger}\rangle}{dt} = i(\omega_1 + \omega_\alpha)\langle a_1^{\dagger}a_\alpha^{\dagger}\rangle + i\sum_{\nu} g_{\nu}\langle (1 - [1 - \varepsilon_1]a_1^{\dagger}a_1)[a_\nu^{\dagger}a_\alpha^{\dagger} + a_\nu a_\alpha^{\dagger}]\rangle + ig_{\alpha}\langle [a_1^{\dagger}a_1 + a_1^{\dagger}a_1^{\dagger}](1 - [1 - \varepsilon_\alpha]a_\alpha^{\dagger}a_\alpha)\rangle,
$$

\n
$$
\frac{d\langle a_\alpha^{\dagger}a_\alpha^{\dagger}\rangle}{dt} = 2i\omega_\alpha\langle a_\alpha^{\dagger}a_\alpha^{\dagger}\rangle + i\frac{1 + \varepsilon_\alpha}{2}g_{\alpha}\langle \langle a_\alpha^{\dagger}a_1\rangle + \langle a_\alpha^{\dagger}a_1^{\dagger}\rangle + \langle a_1a_\alpha^{\dagger}\rangle + \langle a_1^{\dagger}a_\alpha^{\dagger}\rangle),
$$

\n
$$
\frac{d\langle a_\alpha^{\dagger}a_\beta^{\dagger}\rangle}{dt} = i(\omega_\alpha + \omega_\alpha)\langle a_\alpha^{\dagger}a_\beta^{\dagger}\rangle + ig_{\alpha}\langle (1 - [1 - \varepsilon_\alpha]a_\alpha^{\dagger}a_\alpha)[a_1^{\dagger}a_\beta^{\dagger} + a_1a_\beta^{\dagger}]\rangle + ig_{\beta}\langle [a_\alpha^{\dagger}a_1^{\dagger} + a_\alpha^{\dagger}a_1](1 - [1 - \varepsilon_\beta]a_\beta^{\dagger}a_\beta)\rangle. \tag{14}
$$

When the system and environment contain only bosons, we have $[1 - \varepsilon_1] = [1 - \varepsilon_\alpha] = 0$ for all α and we recover the set of equations [\(8\)](#page-2-0). The evolution of the occupation number M_{11} depends on the off-diagonal elements $M_{1\nu}$, $M_{\nu 1}$, $K_{1\nu}$, and $K_{1\nu}^*$ of the normal and anomalous densities whose evolutions depend on $\langle a_1^\dagger a_1 a_\nu^\dagger a_\alpha \rangle$, $\langle a_1^\dagger a_1 a_\nu a_\alpha \rangle$, $\langle a_\alpha^\dagger a_\alpha a_1^\dagger a_1^\dagger \rangle$, $\langle a_\alpha^\dagger a_\alpha a_1^\dagger a_1 \rangle$,.... These degrees of freedom are themselves coupled to higherorder moments related to higher-order quantum fluctuations. The full problem cannot be solved exactly, due to the number of degrees of freedom that should be followed in time when fermions are considered.

If the system is driven by the fermionic and/or bosonic harmonic potentials that destroy high-order quantum fluctuations, then these fluctuations are presented as a product of two diagonal elements or a product of diagonal $(M_{11}, M_{\alpha\alpha}, K_{11},$ $K_{\alpha\alpha}$) and off-diagonal ($M_{\nu\alpha}$, $K_{\alpha\nu}^*$, $K_{\nu\alpha}$, where $\alpha \neq \nu$) elements of the normal and anomalous densities,

$$
\langle a_1^{\dagger} a_1 a_v^{\dagger} a_{\alpha} \rangle \simeq \langle a_1^{\dagger} a_1 \rangle \langle a_v^{\dagger} a_{\alpha} \rangle = M_{11} M_{\nu \alpha},
$$

$$
\langle a_1^{\dagger} a_1 a_v a_{\alpha} \rangle \simeq \langle a_1^{\dagger} a_1 \rangle \langle a_v a_{\alpha} \rangle = M_{11} K_{\alpha \nu}^*,
$$

 $\langle a_{\alpha}^{\dagger}a_{\alpha}a_{1}^{\dagger}a_{1}^{\dagger}\rangle \simeq \langle a_{\alpha}^{\dagger}a_{\alpha}\rangle \langle a_{1}^{\dagger}a_{1}^{\dagger}\rangle = M_{\alpha\alpha}K_{11},$ $\langle a_{\alpha}^{\dagger}a_{\alpha}a_{\alpha}^{\dagger}a_{1}\rangle \simeq \langle a_{\alpha}^{\dagger}a_{\alpha}\rangle\langle a_{1}^{\dagger}a_{1}\rangle = M_{\alpha\alpha}M_{11},$ \cdots (15)

This truncation procedure is equivalent to the linearization of the equations of motion with respect to the off-diagonal elements $M_{\alpha\beta}$, $K_{\alpha\beta}$, $K_{\alpha\beta}^*$ ($\alpha \neq \beta$, including the cases of $\alpha =$ 1, $\beta = 1$). The right-hand sides of these equations contain the terms with the off-diagonal elements only in the first order, i.e., the terms containing a product of two off-diagonal elements are neglected, since they are very small with respect to the corresponding terms that are proportional to a product of two diagonal elements or a product of diagonal and offdiagonal elements.

Employing the mean-field type approximation (15) , we obtain from the exact Eqs. (14) the closed set of equations of motion:

$$
\frac{dM_{11}}{dt} = i \sum_{v} g_{v} (M_{v1} - M_{1v}) + i \sum_{v} g_{v} (K_{1v}^{*} - K_{1v}),
$$
\n
$$
\frac{dM_{1\alpha}}{dt} = i(\omega_{1} - \omega_{\alpha}) M_{1\alpha} + i\xi_{1}(t) \sum_{v} g_{v} (M_{v\alpha} + K_{\alpha v}^{*}) - i g_{\alpha} \xi_{\alpha}(t) (M_{11} + K_{11}),
$$
\n
$$
\frac{dM_{\alpha\alpha}}{dt} = i g_{\alpha} (M_{1\alpha} - M_{\alpha 1} + K_{\alpha 1}^{*} - K_{\alpha 1}),
$$
\n
$$
\frac{dM_{\alpha\beta}}{dt} = i(\omega_{\alpha} - \omega_{\beta}) M_{\alpha\beta} + i g_{\alpha} \xi_{\alpha}(t) (M_{1\beta} + K_{\beta 1}^{*}) - i g_{\beta} \xi_{\beta}(t) (M_{\alpha 1} + K_{\alpha 1}),
$$
\n
$$
\frac{dK_{11}}{dt} = 2i\omega_{1} K_{11} + i \frac{(1 + \varepsilon_{1})}{2} \sum_{v} g_{v} (K_{v1} + M_{1v} + G_{v1} + K_{1v}),
$$
\n
$$
\frac{dK_{1\alpha}}{dt} = i(\omega_{1} + \omega_{\alpha}) K_{1\alpha} + i\xi_{1}(t) \sum_{v} g_{v} (G_{v\alpha} + K_{v\alpha}) + i g_{\alpha} \xi_{\alpha}(t) (M_{11} + K_{11}),
$$
\n
$$
\frac{dK_{\alpha\alpha}}{dt} = 2i\omega_{\alpha} K_{\alpha\alpha} + i \frac{(1 + \varepsilon_{\alpha})}{2} g_{\alpha} (M_{\alpha 1} + K_{\alpha 1} + G_{1\alpha} + K_{\alpha 1}),
$$
\n
$$
\frac{dK_{\alpha\beta}}{dt} = i(\omega_{\alpha} + \omega_{\beta}) K_{\alpha\beta} + i g_{\alpha} \xi_{\alpha}(t) (G_{1\beta} + K_{1\beta}) + i g_{\beta} \xi_{\beta}(t) (M_{\alpha 1} + K_{\alpha 1}),
$$

where $\xi_{\alpha}(t) = \langle [a_{\alpha}, a_{\alpha}^{\dagger}] \rangle$ (including the case of $\alpha = 1$). This set of equations is the main result of the present work. It can be applied regardless of the quantum natures of the system or baths (fermionic or bosonic) as well as to the system coupled to several baths. In the following, the method will be called coupled equations of motion (CEM) method.

There are a number of properties of *M*, *G*, and *K* components which help us to solve these equations. Assuming that each bath is composed of a set of independent two-level systems, we have for all α and β :

$$
K_{\alpha\beta} = K_{\beta\alpha},
$$

\n
$$
G_{\alpha\beta} = M_{\beta\alpha} \quad (\alpha \neq \beta),
$$

\n
$$
G_{\alpha\alpha} = 1 + \varepsilon_{\alpha} M_{\alpha\alpha}.
$$

The last relation implies that we also have $\xi_{\alpha}(t) = 1 + [\varepsilon_{\alpha} 1$ *M*_{αα}.

When the system and baths are all composed of bosons, we have $\xi_1(t) = 1$ and $\xi_\alpha(t) = 1$ for all α and it could be easily shown that Eqs. (16) are reduced to Eqs. (8) . Therefore, we also obtain an exact solution of the problem in the B-B case. Another important property visible in (16) is that, if we assume α to be fermionic, we have simply $K_{\alpha\alpha} = 2i\omega_{\alpha}K_{\alpha\alpha}$. Since at initial time $K_{\alpha\alpha}(0) = 0$ for fermions, this property is also respected at all times as it should be.

The truncation procedure leading to the set of coupled equations [\(16\)](#page-4-0) was tested for the F-F, F-B, and B-F cases. We found that, for these systems, the occupation numbers M_{11} calculated with (16) and within the Langevin approach of Refs. [\[21–27\]](#page-11-0), taking into account the Pauli principle, have almost the same time dependencies and asymptotic values. This indirectly justifies our truncation procedure.

IV. APPLICATIONS

A. System coupled to single heat bath

In the following, the results obtained for the FC Hamiltonian using the CEM approach for a system coupled to one bath with various quantum statistics are compared with our previous calculations in Fig. [1](#page-1-0) for the B-B and F-F and in Fig. [2](#page-3-0) for the B-F and F-B cases.

There are a number of remarks that can be made from the comparison. Since Eqs. (16) are identical to Eqs. (8) in the B-B case, we obviously observe in Fig. [1](#page-1-0) [panels (a) and (c)] that results of the two sets of equations coincide. In all cases, we see in Figs. [1](#page-1-0) and [2](#page-3-0) that the timescale to reach the asymptotic equilibrium is compatible with our previous estimates. However, when fermions are present in the system and/or bath, the amplitudes of oscillation during the descent to equilibrium are reduced in our approach. This is particularly visible when the system is fermionic where the oscillations completely disappear. The asymptotic limit is more modified in the F-B or B-F case (Fig. [2\)](#page-3-0) and to a lesser extent in the F-F case (Fig. [1\)](#page-1-0). When the system is fermionic, we see by comparing Figs. [1](#page-1-0) and [2](#page-3-0) that the quantum nature (fermionic or bosonic) of the bath affects the evolution much less compared to the case of a bosonic system. This will be systematically observed in all illustrations given below. Another generic feature is the absence of unphysical values for the occupation probabilities of a fermionic system when Eqs. [\(16\)](#page-4-0) are solved. This gives indirect indication that the fermionic nature of the system is properly accounted for.

B. Toward simplified treatments of a fermionic or bosonic system coupled to a single heat bath

We propose here a method to treat the Fermi (or Bose) systems coupled to one or several heat baths by solving discretized versions of different heat baths together with numeri-

FIG. 3. Comparison of the evolution of $n_1(t)$ in the FC coupling for a system coupled to a single bath obtained within the CEM approach (black solid lines) at $T_1/\Omega = 2$ (left panels) and $T_1/\Omega = 5$ (right panels). Results are systematically compared to the CEM approach assuming $K_{\alpha\beta} = 0$ and $M_{\alpha\beta} = 0$ for $\alpha \neq \beta$ during the evolution (red dashed line). Here, α and β belong to the bath. The combinations of the system and heat bath are indicated in each panel. All calculations are performed at $\gamma_1/\Omega = 12$ and $c_1 = 0.1$.

cal integration of a closed set of equations between the normal and anomalous densities of the system+environment. The discretization technique can be rather costly numerically. With the aim to treat more elaborated systems (with many qubits) coupled to many heat baths, we further explore the possibility to obtain a simpler framework compared to Eqs. [\(16\)](#page-4-0).

One possibility is to assume that the off-diagonal matrix elements $M_{\alpha\beta}$ and $K_{\alpha\beta}$ in Eqs. [\(16\)](#page-4-0) are zero when both α and β belong to the bath. This approximation, that is expected to be accurate in the weak-coupling regime, is discussed in more details in the Appendix [A.](#page-9-0) In particular, a connection with the diffusion equation [\(13\)](#page-3-0) is made. We compare in Fig. 3 the full and approximate treatments for the F-F, F-B, B-F, and B-B cases. We clearly see from this figure that the approximation leads to unphysical occupation numbers for the bosonic system. Surprisingly enough, for Fermi systems, although not perfect, the approximation turns out to reproduce quite well the full evolution whatever is the nature of the bath. We finally also checked numerically for the F-F case that the approximation is better when the temperature increases but degrades when the coupling strength increases. The same conclusion can be drawn for a Fermi system coupled to several baths independent of the quantum nature of the baths.

FIG. 4. Comparison of the evolution of $n_1(t)$ in the FC coupling for the system coupled to a single bath obtained within the CEM approach (black solid lines) at $T_1/\Omega = 2$ (left panels) and $T_1/\Omega = 5$ (right panels). Results are systematically compared to the CEM approach assuming that the anomalous density is zero $(K = 0)$ together with $M_{\alpha\beta} = 0$ for $\alpha \neq \beta$ during the evolution (red dashed line). Here, α and β belong to the bath. The combinations of the system and heat bath are indicated in each panel. All calculations are performed at $\gamma_1/\Omega = 12$ and $c_1 = 0.1$.

We explored the possibility to obtain the alternative simplified description of a bosonic system coupled to a bosonic or fermionic system. For the bosonic case, one cannot set only part of the anomalous density K to zero. As clearly seen in Eqs. [\(16\)](#page-4-0), this comes from the coupling between the diagonal and off-diagonal matrix elements. For the fermionic case, the situation is different because the diagonal part of *K* is automatically zero. When we neglect only part of the components of *K* for the boson system, we obtain unphysical results. As an alternative to the previous approximation for the boson system, one can also set all components of *K* to zero together with $M_{\alpha\beta} = 0$ if α and β are both in the environment. We compare in Fig. 4 the approximate evolution with the full CEM evolution. By setting $K = 0$, the unphysical evolution observed in Fig. [3](#page-5-0) for the bosonic system disappears. We see that such an approximation is satisfactorily reproducing the asymptotic behavior but some important physics is missed during the evolution to equilibrium. Note that this approximation can also be applied to the Fermi system (Fig. 4) but the reproduction of the full CEM approach degrades compared to the red lines in Fig. [3.](#page-5-0)

In the present section, we discussed the possibility to simplify the description of Fermi-Bose systems coupled to an

FIG. 5. Evolution of $n_1(t)$ obtained in the FC case for the Fermi system coupled to two fermionic baths (a) (notation $F-F_1-F_2$) and for the Bose system coupled to two bosonic baths (b) (notation $B - B_1 - B_2$) using the CEM approach. Two baths have the same temperature $T_1/\Omega = T_2/\Omega = 1$ and the same coupling strengths $c_1 = c_2 = 0.1$. The blue solid line corresponds to $\gamma_1/\Omega = \gamma_2/\Omega = 12$, while the red dashed line is obtained at $\gamma_1/\Omega = 12$ and $\gamma_2/\Omega = 20$.

environment by neglecting the components of the normal $M_{\alpha\beta}$ and anomalous $K_{\alpha\beta}$ densities when α and β are both in the environment in accordance with the eigenstate thermalization hypothesis (ETH) [\[37–43\]](#page-11-0). It would be interesting to investigate further possible connection with the ETH and its domain of different regimes of validity when the quantum nature of the system changes from fermions to bosons.

C. Results for a system coupled with two heat baths

Besides the possibility to treat a mixture of fermions and bosons, one of the attractive aspects of the present method is the possibility to treat the coexistence of several baths. Equations [\(16\)](#page-4-0) to be solved are unchanged when considering several baths. The main difference is the sizes of the *M* and *K* matrices that both increase with the number of baths after discretizing each environment. We consider below a two-level system coupled to two baths. Each bath, discretized using the method presented in Sec. [II B](#page-2-0) (see also [\[24\]](#page-11-0)), is characterized by the parameters c_i and γ_i as well as its initial temperature T_i $(i = 1, 2)$.

1. System coupled to two heat baths of the same quantum nature

As the first illustration, we consider the same conditions as in Ref. [\[21\]](#page-11-0) where the system is coupled to several heat baths of the same quantum nature, i.e., the $F-F_1-F_2$ and $B-B_1-B_2$ cases. These two cases are presented in Fig. 5 and can be compared to Fig. [3](#page-5-0) of Ref. $[21]$. For the B-B₁-B₂ case, we again perfectly recover our previous result. This could be

FIG. 6. Evolution of $n_1(t)$ for the F-F₁-F₂ (black solid line), $B-B_1-B_2$ (green dashed line), $F-B_1-F_2$ (red dotted line), $B-F_1-B_2$ cases (blue dotted-dashed line), $F-B_1-B_2$ (cyan long-dashed line), and B-F1-F2 (pink short dashed-dotted line) obtained with the CEM approach and FC coupling starting from $n_1(0) = 0$ (a) and $n_1(0) = 1$ (b). The coupling strengths, spectral properties, and temperatures are set to $c_1 = c_2 = 0.1$, $\gamma_1/\Omega = 10$, $\gamma_2/\Omega = 15$, $T_1/\Omega = 1$, and $T_2/\Omega = 2.0$. In panel (b), the results for the F-B₁-F₂, F-B₁-B₂, and $F-F_1-F_2$ cases are almost identical.

considered as a numerical test because the Laplace transform method used in Ref. [\[21\]](#page-11-0) and the present approach based on Eqs. [\(16\)](#page-4-0) are strictly equivalent and exact.

For the case of a fermionic system coupled to two fermionic baths, some differences are observed with [\[21\]](#page-11-0), although the global shape and asymptotic limit are similar. In general, while the timescale before reaching equilibrium and the asymptotic limit is globally in agreement with Ref. [\[21\]](#page-11-0), a difference is the absence of oscillations during the thermalization process. We also checked numerically, as was analytically proved in our previous work, that the system coupled to two identical baths (the same γ_i and the same temperature) can be treated as the system coupled to the single bath but with coupling strength equal to $c = c_1 + c_2$.

2. System coupled to two heat baths of mixed quantum natures

We now analyze the change in the evolution compared to the previous case when one of the baths or both baths have different quantum natures compared to the system. Such situations are illustrated in Fig. 6. To uncover the effect of changing fermion into boson or vice versa, we compare situations where all other parameters are unchanged, i.e., spectral function parameters, coupling strength, and bath temperature remain the same.

The first conclusion one could draw from Fig. 6 is that, for the Fermi system, the nature of the heat bath does not affect its evolution much. This is clearly the opposite of the bosonic

system for which replacing the bosonic bath by the fermionic bath induces significant modification both in the intermediate time evolution and asymptotic limit reached by the occupation probability.

Another aspect, which is visible in Fig. 6, is that an asymptotic stationary limit is always reached whatever the nature of the system and heat baths. This is in particular the case for the fermionic system coupled to two baths, one fermionic and one bosonic. The convergence towards the stationary limit is systematically observed whatever the properties of the baths, i.e., when changing the coupling strength, the spectral properties, and/or temperatures of two heat baths. This conclusion is different from the one we obtained previously for the $F-B_1-F_2$. Using a slightly different approximation, we have shown that a stationary solution might never be reached [\[26\]](#page-11-0). It should be noted however that both our previous prescriptions to the problem [\[21,22,25–27\]](#page-11-0) and the present one are only approximate when fermions are considered either in the system and/or baths. The approach proposed here has however the advantage to account properly for the Pauli principle for fermions. This could also be seen from the occupation that remains bounded between 0 and 1. The possibility to reach or not a stationary limit when mixing baths with different quantum natures is an interesting aspect. In particular, dedicated experiments would be interesting to clarify this issue.

Because the bosonic systems coupled to one or several baths have been extensively investigated in our previous studies $[21-27]$, in the following, we focus on the Fermi systems and study in more detail the evolutions obtained with the approach proposed here.

D. Detailed study of a Fermi system coupled to one or two bosonic and*/***or fermionic heat baths**

We systematically use Eqs. (16) to simulate the evolution of the Fermi two-level system coupled to one or two baths at various couplings, thermal, and spectral properties. As illus-trated in Figs. [5](#page-6-0) and 6, the evolution of $n_1(t)$ is rather simple and seems to correspond to the decay process. Based on this observation and with the goal to infer generic properties of the system evolution due to the surrounding environment, we fit the occupation number evolution $n_f(t) = n_1(t)$ with the simple function

$$
n_f(t) = n_f(\infty) + [n_f(0) - n_f(\infty)]e^{-\Gamma_f t}.
$$
 (17)

In the following study, we will consider the case $n_f(0) = 1$. $n_f(\infty)$ and Γ_f are fitted on the evolutions and correspond respectively to the asymptotic occupation number and to the decay time $\tau_f = 1/\Gamma_f$. Despite its simplicity, Eq. (17) turns out to provide a rather precise description of the evolution for the whole range of couplings and temperatures considered. The systematic evolutions of Γ_f and $n_f(\infty)$ obtained in the presence of one or two baths are reported in Fig. [7.](#page-8-0)

Focusing first on the single bath case, we observe that the F-F and F-B cases lead to rather similar properties at low temperature. The evolutions of the Fermi systems at low temperature $(T/\Omega < 1)$ appear to be rather insensitive to the quantum nature of the bath and/or if one or several baths are coupled to the system. When the temperature of the bath(s)

FIG. 7. Evolution of $n_f(\infty)$ (a) and Γ_f (b) obtained by fitting the evolution of $n_f(t)$ with expression [\(17\)](#page-7-0) for the Fermi system coupled to one or two baths with various initial temperatures. The blue circles correspond to the F-F case, where the bath properties are set to $c_1 = 0.1$ and $\gamma_1/\Omega = 12$. The red squares correspond to the F-B case where the only difference with the previous case is that the Fermi bath is replaced by the Bose bath. The green stars correspond to the F-B₁-F₂ case with $c_1 = c_2 = 0.05$, and $\gamma_1/\Omega = \gamma_2/\Omega = 12$. Note the $F-B_1-B_2$ and $F-F_1-F_2$ (not shown) match exactly the $F-B$ and F-F case with a coupling equal to $c_1 + c_2$. In the multibaths case, we assume that all baths are at the same temperature, $T_1 = T_2 = T$. In both panels, the inset is a focus on the low-temperature limit. The green open squares correspond to the result of Eq. (18).

increases, we see significant differences in Γ_f and to a lesser extent in $n_f(\infty)$ depending on the quantum nature of the baths. For $n_f(\infty)$, we see only small differences between the F-F and F-B cases. It is interesting however to mention that the asymptotic occupation number of the $F-B_1-F_2$ matches the one of the F-B case for all temperatures. Therefore, for two baths with different quantum natures but with equivalent spectral properties, the bosonic bath seems to decide the asymptotic behavior.

In the F-F case, the decay time is almost independent of the temperature while, for the F-B case, Γ_f linearly increases with temperature at $T/\Omega > 1$. This implies that the transient time to equilibrium is much shorter if the fermionic system is coupled to a bosonic bath rather than to a fermionic bath. We also observe in Fig. 7 that Γ_f obtained for the F-B₁-F₂ case is in between the F-F and F-B cases. More precisely, we have $\Gamma_f = (\Gamma_{FF} + \Gamma_{FB})/2$, where we use the notations Γ_{FF} (Γ_{FB}) for the value of Γ_f obtained in the F-F (F-B) case. We further investigated this simple behavior in the $F-B_1-F_2$ case by varying the coupling values of c_1 and c_2 , while keeping $c_1 + c_2 = 0.1$. The evolution of Γ_f is displayed as a function

FIG. 8. Evolution of Γ_f obtained for the F-B₁-F₂ as a function of $c_1/(c_1 + c_2)$ assuming that $c_1 + c_2 = 0.1$. The structural properties of the two baths are the same as in Fig. 7, while $T_1/\Omega = T_2/\Omega$ 5. The stars at the extremes correspond to the reference F-F (F-B) calculations put artificially at $c_1/(c_1 + c_2) = 1$ (0). The dashed line is a linear interpolation between the two stars.

of $c_1/(c_1 + c_2)$ in Fig. 8 at $T_1/\Omega = T_2/\Omega = 5$. We observe in this figure that we have approximately

$$
\Gamma_f \simeq \frac{c_1}{(c_1 + c_2)} \Gamma_{\text{FF}} + \frac{c_2}{(c_1 + c_2)} \Gamma_{\text{FB}},
$$
 (18)

which is a very simple relationship.

Note that, if we change the temperature, we change the absolute value of the dependence presented in Fig. 8, but all conclusions remain valid. Such a behavior can again be tested in the experimental observations. In particular, one might imagine by mixing several baths and changing the relative strengths of the couplings with the system to control the decay properties even if the temperatures of different baths are kept fixed.

The approximate treatment of an open quantum Fermi system discussed in Sec. [IV B](#page-5-0) and the Appendix [A](#page-9-0) turns out to be useful to understand qualitatively the conclusion made from Figs. 7 and 8. We have checked numerically that the approximation is also accurate when the Fermi system is coupled to several baths in the high-temperature–weak-coupling limit. As shown in the Appendix [A,](#page-9-0) the simple linear relation (18) can be explained consistently with this simplification. Indeed, starting from the analytical equations $(A9)$ for the asymptotic occupation probability and decay time, one can explain why the decay time is independent of temperature in the case of the Fermi bath, while it increases with the temperature for the Bose bath.

V. CONCLUSION

We proposed here an approach called CEM to describe the single fermionic or bosonic oscillator coupled to one or several baths eventually mixing different quantum natures of the particles (fermions or bosons). The approach is exact when only bosonic degrees of freedom are considered and provide an approximate solution when fermions are also present either in the system and/or in the bath. In this approach, a particular attention is paid to properly account for the Pauli principle for the fermions. The approach is illustrated for the system coupled to a single bath where the system or bath can be either fermionic or bosonic. For Fermi systems, we showed that the

proper treatment of the Fermi nature is essential to obtain an accurate treatment of the evolution.

The approach includes non-Markovian effects and is rather versatile and we do not anticipate any specific difficulty in applying it to the baths with complex structure. We illustrated the method for a system coupled to two baths with various quantum statistics. One of the important aspects that differs from our previous solution $[26,27]$ to this problem is that Fermi systems coupled to two baths always reach an asymptotic stationary limit. Since in the present work, similar to Ref. $[26]$, the approach we propose is not exact, the existence or not of an asymptotic time-independent solution is an interesting debate. In particular, it would be interesting to give an experimental clarification to this aspect. Besides the asymptotic behavior, we observe that Fermi systems have relatively simple decay properties compared to boson systems coupled to the same baths. We showed that the decay time of the Fermi system coupled to the fermionic and bosonic baths can be easily related to the cases of the system coupled to only one bosonic bath or to only one fermionic bath.

In the present work, we focused our attention on a single qubit coupled to a set of environments including fully non-Markovian effects. The theory can *a priori* be extended to obtain numerical simulation of an ensemble of qubits with the price of increasing the numerical cost. With the target goal to be able to treat eventually several hundreds of qubits we also explore the possibility to obtain simplified theories of Fermi systems while not degrading the description of evolution. We show that, in some regime of coupling or temperature, the simplification can indeed be made.

ACKNOWLEDGMENTS

The IN2P3(France)-JINR(Dubna) Cooperation Programme is gratefully acknowledged. This work was partially supported by Russian Foundation for Basic Research (Moscow), Grants No. N 17-52-12015 and No. 20-02-00176. This project has received financial support from the CNRS through the 80Prime program.

APPENDIX: SIMPLIFIED FORM OF EQUATIONS OF MOTION FOR A FERMI SYSTEM COUPLED TO ONE OR SEVERAL BATHS

We consider here the case of a Fermi system coupled to one or several baths. Assuming $K_{\alpha\beta}(t) = M_{\alpha\beta}(t) = 0$ when α and β components are in the bath with $\alpha \neq \beta$ and introducing the notations

$$
n_{\alpha}(t) = M_{\alpha\alpha}(t), \quad \bar{n}_{\alpha}(t) = 1 + \varepsilon_{\alpha} n_{\alpha}(t), \tag{A1}
$$

Eqs. [\(16\)](#page-4-0) are simplified as

$$
\dot{n}_1(t) = i \sum_{\nu} g_{\nu} (M_{\nu 1} - M_{1\nu}) + i \sum_{\nu} g_{\nu} (K_{1\nu}^* - K_{1\nu}),
$$

\n
$$
\dot{n}_{\alpha}(t) = i g_{\alpha} (M_{1\alpha} - M_{\alpha 1}) + i g_{\alpha} (K_{1\alpha}^* - K_{1\alpha}),
$$

\n
$$
\dot{M}_{1\alpha} = i(\omega_1 - \omega_\alpha) M_{1\alpha} + i g_{\alpha} [\bar{n}_1(t) n_\alpha(t) - n_1(t) \bar{n}_\alpha(t)],
$$

\n
$$
\dot{K}_{1\alpha} = i(\omega_1 + \omega_\alpha) K_{1\alpha} + i g_{\alpha} [\bar{n}_1(t) \bar{n}_\alpha(t) - n_1(t) n_\alpha(t)].
$$
\n(A2)

The numerical integration of these equations of motion is much less demanding than the original set of equations [\(16\)](#page-4-0). This could be seen from the fact that the original number of coupled equations was $2N_{\text{tot}}^2$, where N_{tot} is the total number of creation and annihilation operators for the system+baths, while the number of coupled equations in $(A2)$ is reduced to $(3N_{tot} - 2)$.

1. Pauli master equation with memory effect

Related approximation has been discussed, for instance, in Refs. [\[21,22\]](#page-11-0). Following these references, one might eventually obtain the closed form of the equations for $n_1(t)$ and $n_\alpha(t)$ by formally integrating the last two equations. Using the fact that $M_{1\alpha}(0) = K_{1\alpha}(0) = 0$, we have the formal solution:

$$
ig_{\alpha}[M_{\alpha 1}(t) - M_{1\alpha}(t)] = 2g_{\alpha}^{2} \int_{0}^{t} \cos([\omega_{1} - \omega_{\alpha}][t - \tau])[\bar{n}_{1}(\tau)n_{\alpha}(\tau) - n_{1}(\tau)\bar{n}_{\alpha}(\tau)],
$$

$$
ig_{\alpha}[K_{1\alpha}^{*}(t) - K_{1\alpha}(t)] = 2g_{\alpha}^{2} \int_{0}^{t} \cos([\omega_{1} + \omega_{\alpha}][t - \tau])[\bar{n}_{1}(\tau)\bar{n}_{\alpha}(\tau) - n_{1}(\tau)n_{\alpha}(\tau)].
$$

The evolution of the system occupation probabilities is written as the Pauli master equation:

$$
\frac{dn_1(t)}{dt} = \int_0^t \left\{ \mathcal{W}_+^1(t, \tau) \bar{n}_1(\tau) - \mathcal{W}_-^1(t, \tau) n_1(\tau) \right\} d\tau,\tag{A3}
$$

with

$$
\mathcal{W}_{+}^{1}(t,\tau) = 2 \sum_{\alpha} g_{\alpha}^{2} [\cos([\omega_{1} - \omega_{\alpha}][t-\tau])n_{\alpha}(\tau) + \cos([\omega_{1} + \omega_{\alpha}][t-\tau])\bar{n}_{\alpha}(\tau)],
$$

$$
\mathcal{W}_{-}^{1}(t,\tau) = 2 \sum_{\alpha} g_{\alpha}^{2} [\cos([\omega_{1} - \omega_{\alpha}][t-\tau])\bar{n}_{\alpha}(\tau) + \cos([\omega_{1} + \omega_{\alpha}][t-\tau])n_{\alpha}(\tau)].
$$

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These expressions can eventually be complemented by the set of equivalent master equations for the $n_{\alpha}(t)$ (not shown here). In the following, we use the notations $G_1(\tau) = \mathcal{W}_+^1(t, \tau) + \mathcal{W}_-^1(t, \tau)$ and $F_1(\tau) = \mathcal{W}_+^1(t, \tau) - \mathcal{W}_-^1(t, \tau)$. Some simple manipulations result in the expressions

$$
G_1(t, \tau) = 4 \cos(\omega_1 \tau) \sum_{\alpha} g_{\alpha}^2 \cos(\omega_{\alpha} \tau) [n_{\alpha}(\tau) + \bar{n}_{\alpha}(\tau)],
$$
\n(A4)

$$
F_1(t, \tau) = 4 \sin(\omega_1 \tau) \sum_{\alpha} g_{\alpha}^2 \sin(\omega_{\alpha} \tau) [n_{\alpha}(\tau) - \bar{n}_{\alpha}(\tau)].
$$
 (A5)

2. Simple approximate form for system evolution in the weak-coupling regime

Starting from the master equation $(A2)$, one might try to see if the equation of motion of the system occupation number can be written in terms of a time-local equation while properly keeping non-Markovian effects. Our goal is to make a connection with the simple form [\(17\)](#page-7-0) used to fit the $n_1(t)$ evolution. For this, we first rewrite the master equation as

$$
\frac{dn_1(t)}{dt} = -\int_0^t G_1(t, \tau) n_1(\tau) d\tau + \int_0^t \mathcal{W}_+^1(t, \tau) d\tau,
$$
\n(A6)

where we use the fact that the system is fermionic. Note that $G_1(t, \tau)$ is linked to the decay time of the Fermi system. If the bath contains only fermions, i.e., for all α we have $n_{\alpha}(\tau) + \bar{n}_{\alpha}(\tau) = 1$, this quantity becomes independent of the initial temperature of the baths. Starting from this expression, using the expression for *g*^α given in Sec. [II B,](#page-2-0) and taking the continuous limit for the bath, we deduce for a fermionic bath

$$
G_1(t,\tau) = 4\cos(\omega_1\tau)\int_0^{+\infty} d\omega J_1(\omega)\cos(\omega\tau), \tag{A7}
$$

where $J_1(\omega)$ is the spectral function [\(9\)](#page-2-0).

From now on, we assume that the coupling between the system and bath is weak enough and we can only retain terms up to the second order in g_{α}^2 . Consistent with this approximation, one might eventually make the replacement $n_1(\tau) \simeq n_1(t)$ together with $n_{\alpha}(\tau) \simeq n_{\alpha}(0)$ in the integral in time such that we obtain

$$
\frac{dn_1(t)}{dt} \simeq -\Gamma_f(t)n_1(t) + D_f(t),\tag{A8}
$$

where we use

$$
\Gamma_f(t) \simeq \int_0^t \overline{G_1}(\tau) d\tau, \quad D_f(t) \simeq \frac{1}{2} \int_0^t \left[\overline{G_1}(\tau) + \overline{F_1}(\tau) \right] d\tau,\tag{A9}
$$

with

$$
\overline{G_1}(\tau) = 4 \cos(\omega_1 \tau) \sum_{\alpha} g_{\alpha}^2 \cos(\omega_{\alpha} \tau) [n_{\alpha}(0) + \bar{n}_{\alpha}(0)],
$$

$$
\overline{F_1}(\tau) = 4 \sin(\omega_1 \tau) \sum_{\alpha} g_{\alpha}^2 \sin(\omega_{\alpha} \tau) [n_{\alpha}(0) - \bar{n}_{\alpha}(0)].
$$

Equations $(A8)$ and $(A9)$ can be generalized to the case of several baths.

From these expressions, we see that $\overline{G_1}(\tau)$ and therefore Γ_f calculated with Eqs. (A9) are independent of temperature for the fermion bath (Fig. [7\)](#page-8-0). However, Γ_f depends on temperature for the bosonic bath.

Note finally that, in the simplified scenario presented here, one deduces a simple time-local equation, valid *a priori* in the weak-coupling regime. This equation however includes partially non-Markovian effects. As a side remark, it would be interesting to investigate the possibility of extending the time-convolutionless approach of Refs. [\[29,44–47\]](#page-11-0) to obtain a systematic constructive framework leading to the time-local equation of motion for the system with higher-order corrections in the coupling.

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