Symmetry and block structure of the Liouvillian superoperator in partial secular approximation

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(Received 19 November 2019; revised manuscript received 4 February 2020; accepted 11 March 2020; published 13 April 2020)

We address the structure of the Liouvillian superoperator for a broad class of bosonic and fermionic Markovian open systems interacting with stationary environments. We show that the accurate application of the partial secular approximation in the derivation of the Bloch-Redfield master equation naturally induces a symmetry on the superoperator level, which may greatly reduce the complexity of the master equation by decomposing the Liouvillian superoperator into independent blocks. Moreover, we prove that, if the steady state of the system is unique, one single block contains all the information about it, and that this imposes a constraint on the possible steady-state coherences of the unique state, ruling out some of them. To provide some examples, we show how the symmetry appears for two coupled spins interacting with separate baths, as well as for two harmonic oscillators immersed in a common environment. In both cases the standard derivation and solution of the master equation is simplified, as well as the search for the steady state. The block diagonalization does not appear when a local master equation is chosen.

DOI: 10.1103/PhysRevA.101.042108

I. INTRODUCTION

Open quantum systems are nowadays a well-established framework whose theoretical aspects have been investigated in depth [1–3]. An important branch is represented by Markovian open systems [4,5] and quantum dynamical semigroups [6]. In particular, the generator of a quantum dynamical semigroup is a time-independent *Liouvillian superoperator* $\mathcal{L}$, such that if $\rho_S(0)$ is the initial state of the system, the state at time t is given by $\rho_S(t) = \exp(\mathcal{L}t)[\rho_S(0)]$. The solution of the master equation providing the dynamics of the system relies on finding the Liouvillian $\mathcal{L}$.

The evolution of a dynamical semigroup is described by a master equation in the so-called Gorini-Kossakowski-Sudarshan-Lindblad (GKLS) form [7–9]. This form has been extensively studied during recent years [10–19], with a particular attention on the steady-state structure, given the importance of, for instance, steady-state coherences in quantum thermodynamics [20–22] or of information-preserving steady states [23]. The form of the steady state is also crucial to understand the process of quantum thermalization [24]. The investigation of the role of symmetry in the semigroup evolution has been very active as well [25–33]. Given the simplicity of the GKLS master equation, a thornier issue has been to characterize which microscopic physical models of systems and environments lead to a reduced system evolution described by this master equation. In 1965 Redfield derived a Markovian master equation by assuming weak coupling between system and environment *and* making some considerations about the relevant timescales of the evolution [34]. This derivation and the subsequent Bloch-Redfield master equation are still commonly employed nowadays [1,2,35]. A more formal derivation has been provided by Davies [36,37], showing that the semigroup evolution is perfectly recovered when the coupling between system and environment is infinitesimally small. In some situations, e.g., in the case of two slightly detuned spins [38,39], the Davies' limit cannot be performed, since it corresponds to applying a "full secular approximation" removing all the oscillating terms in the interaction picture dynamics without discriminating which of them are fast and which are slow, instead of a more accurate partial secular approximation. The latter was implicitly suggested by Redfield himself [34], and an extensive study about it has been performed in the very recent past [35,39–43], in particular showing that applying an accurate partial secular approximation to the microscopic derivation of the master equation allows one to recover the GKLS form [40,41].

In this work we show how a symmetry on the superoperator level arises due to the partial secular approximation. Our discussion is valid for a broad class of systems that can be recast as M noninteracting fermionic or bosonic modes weakly coupled to stationary Markovian environments. The symmetry consists of the invariance of the Liouvillian superoperator under the action of the total-number-of-particles superoperator. We stress that the symmetry is on the superoperator level, i.e., it is not a symmetry of the system Hamiltonian, but of the full master equation of the open system. Following the formalism discussed in Ref. [27], we can exploit it to block diagonalize the Liouvillian superoperator and greatly reduce the complexity of the master equation. Complexity reduction of abstract GKLS master equations in fermionic or bosonic systems has been also addressed in some extensive works by

Prosen *et al.* [12,14,15], while Torres exploited a symmetry of the Hamiltonian to find the solution of master equations without gain [44]. Once having exploited the symmetry to obtain the block diagonalization, we observe that, if the steady state of the system is unique, one single block contains all the information about it. This not only helps to find it, but also imposes a constraint on the corresponding steady-state coherences. Curiously, the symmetry arises only when considering a global master equation, while it is not valid anymore when using a local one [39,45,46].

We review the derivation of the Bloch-Redfield master equation and subsequent partial secular approximation in Sec. II, as well as the theory of symmetries and conserved quantities in Lindblad master equations. Section III is devoted to the discussion of the symmetry on the superoperator level and to the block diagonalization of the Liouvillian. In particular, Sec. III A discusses the class of systems for which our analysis is valid, while Sec. III B presents the main result and Sec. III C its consequences. We provide some illustrative examples of the action of the symmetry in Sec. IV, distinguishing between fermionic and bosonic scenarios. Finally, we conclude in Sec. V with a discussion about our results.

II. FORMAL FRAMEWORK

A. Markovian master equations with partial secular approximation

Let us consider an open quantum system S with associated Hilbert space H_S of dimension N, described at time t by the $N \times N$ density matrix $\rho_S(t)$. S is coupled to an external environment E through the interaction Hamiltonian $\hat{H}_I$, and throughout the work we restrict ourselves to stationary environments. The full system-bath Hamiltonian can be written as

$$\begin{aligned}\hat{H} &= \hat{H}_S + \hat{H}_E + \hat{H}_I \\ &= \hat{H}_S + \hat{H}_E + \mu \sum_\alpha \hat{A}_\alpha \otimes \hat{B}_\alpha,\end{aligned} \tag{1}$$

where $\hat{H}_S$ is the free Hamiltonian of the system, $\hat{H}_E$ is the free Hamiltonian of the environment, $\hat{A}_\alpha$ are system operators, while $\hat{B}_\alpha$ are bath operators. μ is a coupling constant with units of energy, and in the weak-coupling limit considered here we assume μ far smaller than the other characteristic energies of the system. We set $\hbar = 1$, so that the units of measure of time are [time] = [energy]$^{-1}$.

We term $|e_n\rangle$ the eigenvectors of the free Hamiltonian of the system, which may be degenerate as well, such that $\hat{H}_S = \sum_n \epsilon_n |e_n\rangle\langle e_n|$. The *jump operators* of the system are defined as [1]

$$\hat{A}_\alpha(\omega) = \sum_{\epsilon_m - \epsilon_n = \omega} |e_n\rangle\langle e_n|\hat{A}_\alpha|e_m\rangle\langle e_m|. \tag{2}$$

We assume that the open system S follows a Markovian, nonunitary evolution due to the coupling to the stationary environment E. The master equation describing a time-independent dynamical semigroup is written as

$$\frac{d}{dt}\rho_S(t) = \mathcal{L}[\rho_S(t)], \tag{3}$$

where $\mathcal{L}$ is the *Liouvillian superoperator* acting on the N^2-dimensional Hilbert space L of the linear operators on H_S, called Liouville space [27], which contains the convex subset of the density matrices. In particular, for the Bloch-Redfield master equation in partial secular approximation (PSA) [1,2,39]:

$$\mathcal{L} = -i[\hat{H}_S + \hat{H}_{\mathrm{LS}}, \cdot\,] + \mathcal{D}[\,\cdot\,], \tag{4}$$

where $\hat{H}_{\mathrm{LS}}$ is the *Lamb-shift Hamiltonian* given by

$$\hat{H}_{\mathrm{LS}} = \sum_{\alpha,\beta} \sum_{(\omega,\omega')\in \mathrm{PSA}} S_{\alpha\beta}(\omega,\omega')\hat{A}_\alpha^\dagger(\omega')\hat{A}_\beta(\omega), \tag{5}$$

while the *dissipator* reads

$$\begin{aligned}\mathcal{D}[\rho_S] = \sum_{\alpha,\beta} \sum_{(\omega,\omega')\in \mathrm{PSA}} &\gamma_{\alpha\beta}(\omega,\omega')(\hat{A}_\beta(\omega)\rho_S\hat{A}_\alpha^\dagger(\omega') \\ &- \frac{1}{2}\{\hat{A}_\alpha^\dagger(\omega')\hat{A}_\beta(\omega), \rho_S\}).\end{aligned} \tag{6}$$

$S_{\alpha\beta}(\omega,\omega')$ and $\gamma_{\alpha\beta}(\omega,\omega')$ are functions of the autocorrelation functions of the bath operators $\hat{B}_\alpha$.[1] The PSA removes all the terms in the summation with frequencies ω and ω' such that

$$\exists\, t^* \text{ such that } |\omega - \omega'|^{-1} \ll t^* \ll \tau_R, \tag{7}$$

where τ_R is the relaxation time of the system, i.e., the time in which ρ_S approaches the dynamical equilibrium [1,39]. We can express Eq. (7) as $|\omega - \omega'| \neq \mathcal{O}_{t^*}(\tau_R^{-1})$, where for convenience we introduce the notation $\mathcal{O}_{t^*}$, defined as

$$x = \mathcal{O}_{t^*}(y) \text{ if } \nexists\, t^* \text{ such that } x^{-1} \ll t^* \ll y^{-1}. \tag{8}$$

In the weak-coupling limit considered here we have

$$\tau_R = O(\mu^{-2}) \tag{9}$$

being the master equation of the second order in μ [3]. Appendix A1 discusses why Eq. (3) with Liouvillian in Eq. (4) can be recast in the GKLS form:

$$\mathcal{L}[\rho_S(t)] = -i[\hat{H}', \rho_S(t)] + \sum_{l=1}^{N^2-1} \hat{F}_l\rho_S(t)\hat{F}_l^\dagger - \frac{1}{2}\{\hat{F}_l^\dagger\hat{F}_l, \rho_S(t)\}, \tag{10}$$

where $\hat{H}' = \hat{H}'^\dagger$ is the effective Hamiltonian including the Lamb shift, and $\{\hat{F}_l\}_{l=1}^{N^2-1}$ are the *Lindblad operators* [1].

From now on we will use calligraphic letters (such as $\mathcal{L}$) to indicate superoperators *acting on* L, while we will use capital letters, with hats when needed to avoid confusion, (such as $\hat{H}$) for operators *living in* L, which for instance may act on the Hilbert space of the system H_S. The density matrices ρ_S are elements of L as well. Appendix A2 discusses the language of superoperators in more detail.

B. Symmetries and conserved quantities in the Lindblad formalism

In this section we introduce the concepts of symmetries and conserved quantities in the Lindblad formalism following the recent work by Albert and Jiang [27]. Let us assume that the

[1] We refer the reader to Ref. [39] for their precise form.

Lindblad evolution of an open system S is described by the Liouvillian superoperator $\mathcal{L}$ as discussed in Sec. II A. Given an observable $\hat{J} = \hat{J}^\dagger$ acting on $\mathsf{H_S}$ and living in L, we have the following definitions:

(1) $\hat{J}$ is a *conserved quantity* if it is a constant of motion under the nonunitary evolution generated by the master equation, i.e., if $\mathcal{L}^\dagger[\hat{J}(t)] = 0$ for all t.

We construct the one-parameter unitary group whose elements are $\hat{U}_\phi = \exp(i\phi\hat{J})$ with $\phi \in \mathbb{R}$, and then we define the associated superoperators $\mathcal{U}_\phi$ as $\mathcal{U}_\phi^\dagger[\hat{O}] = \hat{U}_\phi^\dagger \hat{O} \hat{U}_\phi$, with $\hat{O} \in \mathsf{L}$. We can analogously write $\mathcal{U}_\phi = \exp(i\phi\mathcal{J})$, where $\mathcal{J}$ is the superoperator associated with $\hat{J}$ through $\mathcal{J} = [\hat{J}, \cdot\,]$. In the language of the isomorphism introduced through the tensor product notation in Appendix A2, we have $\mathcal{J} = \hat{J} \otimes \mathbb{I}_N - \mathbb{I}_N \otimes \hat{J}^T$.

(2) $\hat{J}$ generates *a continuous symmetry on the superoperator level* if $\mathcal{U}_\phi^\dagger \mathcal{L} \mathcal{U}_\phi = \mathcal{L}$ for all ϕ, or equivalently $[\mathcal{J}, \mathcal{L}] = 0$. The continuous symmetry is also called *covariance* [47–49], given that it corresponds to the equivalence $\hat{U}_\phi^\dagger \mathcal{L}[\rho_S]\hat{U}_\phi = \mathcal{L}[\hat{U}_\phi^\dagger \rho_S \hat{U}_\phi]$, for any state of the system ρ_S.

If the evolution of the system were unitary and driven only by the Hamiltonian $\hat{H}_S$, according to Noether's theorem a conserved quantity would always generate a symmetry and vice versa. In the framework of open systems this is no longer true, since for instance a symmetry on the superoperator level not always implies a symmetry on the operator level. In particular, if the master equation is in the Lindblad form as in Eq. (10), we can consider the following three propositions:

(i) $[\hat{J}, \hat{H}'] = [\hat{J}, \hat{F}_l] = 0 \quad \forall\, l$,
(ii) $\frac{d}{dt}\hat{J}(t) = \mathcal{L}^\dagger[\hat{J}(t)] = 0$,
(iii) $\mathcal{U}_\phi^\dagger \mathcal{L} \mathcal{U}_\phi = \mathcal{L}\ \forall \phi \in \mathbb{R}$, or equivalently $[\mathcal{J}, \mathcal{L}] = 0$.

Then we have that (i) implies (ii) and (iii), but no other logical implications are present [27]. This tells us that an observable $\hat{J}$ may be a conserved quantity but not generate a symmetry on the superoperator level, and vice versa.

For the purpose of this paper we are interested in the observable representing the total number of particles in a system: suppose we have a system of M bosonic or fermionic modes; then the Hilbert space of the system is the tensor product of the Hilbert spaces of the M modes. The total-number-of-particles operator reads

$$\hat{N} = \sum_{k=1}^{M} \hat{n}_k, \tag{11}$$

where $\hat{n}_k$ is the particle number operator of the kth mode. $\hat{N}$ generates the one-parameter group $\hat{U}_\phi = \exp(i\phi\hat{N})$. If we set $\phi = \pi$, we obtain the *parity operator*:

$$\hat{P} = \exp(i\pi\hat{N}). \tag{12}$$

The parity operator satisfies the properties $\hat{P}^2 = \mathbb{I}$ and $\hat{P}^\dagger = \hat{P}$, and as a consequence it only has two eigenvalues, ± 1. Parity is an observable which can generate a *discrete* symmetry on the superoperator level.[2] In analogy with the definition of a continuous symmetry, we write the parity superoperator as

$$\mathcal{P} = \exp(i\pi\mathcal{N}), \tag{13}$$

where $\mathcal{N}$ is defined as

$$\mathcal{N} = [\hat{N}, \cdot\,]. \tag{14}$$

Equivalently, using the tensor product notation (see Appendix A2) we have

$$\mathcal{N} = \hat{N} \otimes \mathbb{I} - \mathbb{I} \otimes \hat{N}^T. \tag{15}$$

Being different objects, symmetries and conserved quantities play a different role in the analysis of the evolution of open quantum systems [10,11,25,27]. Conserved quantities are of fundamental importance to identify the structure of the space of stationary states of the systems [27], related to the problem of finding decoherence-free subspaces [50]. Symmetries can help in simplifying the form of the Liouvillian superoperator, and thus in solving the master equation. Indeed, if we identify a symmetry such that $[\mathcal{J}, \mathcal{L}] = 0$, we can block diagonalize the Liouvillian with each block labeled by a different eigenvalue of $\mathcal{J}$. As we will see in the next section, this can greatly reduce the complexity of the master equation.

III. THE BLOCK STRUCTURE OF THE LIOUVILLIAN IN PARTIAL SECULAR APPROXIMATION

In this section we will show how, for a broad class of models, the partial secular approximation naturally induces a symmetry on the superoperator level, which can be exploited to simplify the master equation. Note that we can apply the concepts of Sec. II B, introduced in the Lindblad formalism, to the Bloch-Redfield master equation in partial secular approximation, since as explained in Appendix A1 the latter can be brought to the GKLS form.

We start by introducing the suitable class of Hamiltonians in Sec. III A, and then we focus on the identification of the symmetry in Sec. III B. Section III C discusses a series of interesting applications and consequences of the main result.

A. Delimiting the suitable class of systems

Our analysis applies to all systems that can be cast as the sum of the free Hamiltonians of M noninteracting bosonic or fermionic modes, with

$$\hat{H}_S = \sum_{k=1}^{M} E_k \hat{c}_k^\dagger \hat{c}_k = \sum_{k=1}^{M} E_k \hat{n}_k, \tag{16}$$

and E_k is the energy quantum of the kth mode.

Equation (16) describes a broad class of Hamiltonians which are particularly relevant in the fields of condensed matter and optical physics. For instance, any quadratic Hamiltonian, that is to say any Hamiltonian of the form

$$\hat{H}_S = \sum_{j,k=1}^{M} (\alpha_{jk}\hat{a}_j^\dagger \hat{a}_k + \beta_{jk}\hat{a}_j\hat{a}_k + \text{H.c.}), \tag{17}$$

where $\hat{a}_j$ is an annihilation operator, can be rewritten as a sum of noninteracting modes as in Eq. (16) [51,52]. This is just a sufficient but not necessary condition, since more complex Hamiltonians may be taken into the form of Eq. (17). In

[2] Discrete symmetries in the Lindblad formalism deserve a separate discussion, and we refer the interested reader to Ref. [27].

the case of bosons, all $\hat{H}_S$ preserving Gaussian states can be recast as Eq. (16). These Hamiltonians contain linear and/or bilinear terms and can be reduced into the form of Eq. (17) through displacement transformations. Systems of uncoupled spins can be trivially seen as noninteracting fermions via Jordan-Wigner transformation [51,53], and thus are suitable for our discussion. The same holds for interacting spin chains in which the total number of spin excitations is conserved (see Appendix C). Two coupled qubits can be transformed into free fermions as well, as discussed in Appendix D, while extensions to wider systems of interacting spins (such as the Heisenberg model) are tricky and must be considered case by case.

We now set the relevant assumptions on the interaction Hamiltonian $\hat{H}_I$ in Eq. (1). First of all, recalling that μ is the system-bath coupling constant defined in Eq. (1), we set $E_k \neq \mathcal{O}_{t^*}(\mu^2)\ \forall\, k$, where we have used the notation introduced in Eq. (8). Then, the interaction Hamiltonian is suitable for our analysis if *at least one* of the following conditions holds:

(i) *Condition I.* Each system operator $\hat{A}_\alpha$ in Eq. (1) involves only single excitations, that is to say, each $\hat{A}_\alpha$ is a first-degree polynomial in the creation and annihilation operators $\hat{c}_k$. For instance, $\hat{A}_{\alpha'} = \hat{c}_1 + \hat{c}_2^\dagger$ is a valid system operator, while $\hat{A}_{\alpha'} = \hat{c}_1\hat{c}_2^\dagger$ or $\hat{A}_{\alpha'} = \hat{c}_1\hat{c}_2$ are not.

(ii) *Condition II.* Let us consider the set of energies $K = \{E_k\}_{k=1}^M$. Create two new sets by randomly selecting some elements of K that can be repeated as well, and term them X and Y; assume that they have different cardinality (number of elements): $|X| \neq |Y|$. Then we exclude situations such that $\sum_{E_m\in X} E_m = \sum_{E_l\in Y} E_l + \mathcal{O}_{t^*}(\mu^2)$. This condition can be relaxed depending on the structure of the system operators in the interaction Hamiltonian, as we will show in the proof in Appendix B. Notice that *condition II* comprises *condition I* together with the assumption $E_k \neq \mathcal{O}_{t^*}(\mu^2)$.

B. The symmetry of the partial secular approximation

We will now show that, if the requirements of Sec. III A are satisfied, the number superoperator $\mathcal{N}$ defined in Eq. (14) commutes with the Liouvillian in partial secular approximation Eq. (4), and therefore generates a symmetry on the superoperator level.

Proposition 1 (Symmetry). Let $\mathcal{L}$ be the Liouvillian superoperator describing the Markovian evolution of a quantum system that can be written as a collection of bosonic or fermionic noninteracting modes. If $\mathcal{L}$ has been derived, starting from the microscopic model of system+environment, through the Bloch-Redfield master equation in partial secular approximation, then it commutes with the number superoperator:

$$[\mathcal{N}, \mathcal{L}] = 0, \tag{18}$$

provided that one of the conditions I or II on the interaction Hamiltonian $\hat{H}_I$ discussed in Sec. III A holds.

Proof. In Appendix B. ■

Note that Proposition 1 may be considered as the extension to systems of M modes of the concept of *phase-covariant master equation* [49,54–56]. By now, the latter has been addressed as the problem in which a system of a single qubit follows an open dynamics described by the Liouvillian $\mathcal{L}$ which is covariant under a phase transformation, i.e., $e^{-i\phi\hat{\sigma}_z}\mathcal{L}[\rho_S]e^{i\phi\hat{\sigma}_z} = \mathcal{L}[e^{-i\phi\hat{\sigma}_z}\rho_S e^{i\phi\hat{\sigma}_z}]$, which corresponds to Eq. (18) in the case of a single fermionic mode. Therefore, the symmetry group generated by $\mathcal{N}$ is isomorphic to U(1). A complete characterization of the single-qubit phase-covariant master equation can be found in the Supplementary Material of Ref. [54].

C. Consequences of the symmetry

In this section we discuss a list of interesting consequences of the symmetry presented in Proposition 1. We start with a simple corollary:

Corollary 1 (Parity). If the conditions for Proposition 1 hold, then the parity superoperator $\mathcal{P}$ is a symmetry on the superoperator level as well: $[\mathcal{P}, \mathcal{L}] = 0$.

Proof. If the conditions for Proposition 1 hold, then $[\mathcal{N}, \mathcal{L}] = 0$. But according to Eq. (13) $\mathcal{P} = \exp(i\pi\mathcal{N})$, thus the parity superoperator must commute with the Liouvillian as well proving the assertion. ■

Notice that the symmetries in Proposition 1 and Corollary 1 are, in general, only on the superoperator level. Indeed, we are not imposing any further condition on the form of the interaction and on the spectral density of environment, that is to say, the result of Eq. (18) is an interesting consequence of the partial secular approximation only. This includes cases in which the parity of the number of particles (on the operator level) is modified by the interaction with the environment. For instance, the very common decay of a single mode of the electromagnetic field, described as $\dot{\rho} = a\rho a^\dagger - 1/2\{a^\dagger a, \rho\}$ [1], clearly does not conserve either $\hat{N}$ or $\hat{P}$, while as it holds the partial secular approximation it fulfils Eq. (18).

How can we exploit Eq. (18) for the analysis of the open system? As already mentioned in Sec. II B, the symmetry generated by the number superoperator allows us to block diagonalize the Liouvillian in a way that is particularly convenient for the solution of the master equation. Indeed, the eigenvectors of $\mathcal{N}$ in the representation expressed by Eq. (15) are given by the tensor product of the diagonal basis of $\hat{H}_S$ with itself. That is to say, if we rewrite the system Hamiltonian as $\hat{H}_S = \sum_n \epsilon_n |e_n\rangle\langle e_n|$, we choose the basis of the space of superoperators $\{|e_n\rangle \otimes |e_m\rangle\}_{n,m}$. This is exactly the basis we work with when deriving the Bloch-Redfield master equation, since it is the basis in which we write the jump operators [1,2,39]. Therefore, if we express $\mathcal{L}$ as a matrix in the basis $|e_n\rangle \otimes |e_m\rangle$, and we regroup all the elements of the basis which are eigenvectors of $\mathcal{N}$ with the same eigenvalue d, we naturally find the blocks of the Liouvillian in such basis. Note that d is the difference between the number of particles in the state $|e_n\rangle$ and the number of particles in $|e_m\rangle$. We can express this fact in the following proposition:

Proposition 2 (Blocks). In a system of M bosonic or fermionic modes in which Proposition 1 holds, the Liouvillian superoperator can be divided into blocks as $\mathcal{L} = \bigoplus_d \mathcal{L}_d$, where $\mathcal{L}_d$ is the block labeled by the eigenvalue d of $\mathcal{N}$. Let us write $\mathcal{L}_d$ as a matrix in a basis $\{|e_j\rangle \otimes |e'_k\rangle\}_{j,k}$ which spans its space, where $|e_j\rangle$ and $|e'_k\rangle$ are eigenvectors of $\hat{H}_S$. Then, if we write $\mathcal{L}_{-d}$ as a matrix in the basis $\{|e'_k\rangle \otimes |e_j\rangle\}_{j,k}$ these matrices satisfy $\mathcal{L}_d = \mathcal{L}_{-d}^*$.

Proof. The Liouvillian can be block diagonalized thanks to the symmetry expressed by Eq. (18), generated by $\mathcal{N}$ whose eigenvalues label the blocks. $\mathcal{L}$ describes the dynamics of the density matrix of the system ρ_S as in Eq. (3), but since $(\rho_S)_{jk} = (\rho_S)^*_{kj}$, we have in the chosen bases $\mathcal{L}_d = \mathcal{L}^*_{-d}$. ■

Proposition 2 tells us that the symmetry in Eq. (18) not only provides a block division for the Liouvillian, but also reduces the number of independent blocks, e.g. for fermions from $2M + 1$ to $M + 1$. This may greatly simplify the solution of the master equation, which now would live in spaces of lower dimension. We will show in Sec. IV some examples of this block diagonalization and complexity reduction.

Each block of the Liouvillian superoperator may give us important insight about a certain physical phenomenon of interest. If we know that a given block contains all the relevant information about such phenomenon, we may indeed analyze only this block and neglect all the rest, thus working in a far smaller space than the one in which $\mathcal{L}$ lives. This happens, for instance, in Ref. [57], where two independent blocks of the Liouvillian superoperator describing the decay of two spins (corresponding to the blocks discussed in Proposition 2) contain all the information about two different physical phenomena, namely superradiance and quantum synchronization. Besides, note that all the populations of the state of the system belong to the block $\mathcal{L}_0$.

Finding the unique steady state of a relaxing Lindblad dynamics is another example of the advantages entailed by the block structure of $\mathcal{L}$: a steady state of the open dynamics is a state ρ_{ss} such that $\mathcal{L}[\rho_{ss}] = 0$. It always exists at least one steady state for finite systems [3,11] and, if it is unique, then the semigroup is relaxing, i.e., any state is driven toward ρ_{ss} for $t \to \infty$, and no oscillating coherence survives.

The unique steady state "lives" in the subspace of the block $\mathcal{L}_0$ only. Indeed, let us call Π_0 the projector over the eigenspace of $\mathcal{N}$ associated with the eigenvalue 0. Then the following proposition holds:

Proposition 3 (Steady state). If the conditions for Proposition 1 hold and the semigroup generated by $\mathcal{L}$ is relaxing toward a unique steady state ρ_{ss}, then $\Pi_0[\rho_{ss}] = \rho_{ss}$. i.e., the only nonzero elements of the density matrix representing ρ_{ss} in the excitation basis are the ones with equal number of excitations in the ket and in the bra.

Proof. Let us suppose that the steady state ρ_{ss} has a nonzero component in a subspace projected by Π_d with $d \neq 0$: $\Pi_d[\rho_{ss}] \neq 0$. Coming back to the space of density matrices, this means that the density matrix of the steady state in the excitation basis has some nonzero elements with different number of particles in the bra and in the ket. Therefore, there exists a block $\mathcal{L}_d$ with $d \neq 0$ having a zero eigenvalue. Furthermore, the block $\mathcal{L}_0$ must have a zero eigenvalue as well, since for ρ_{ss} to be a physical state it must possess diagonal elements. We now build a new state ρ'_{ss} such that $\Pi_0[\rho'_{ss}] = \Pi_0[\rho_{ss}]$ and $\Pi_k[\rho'_{ss}] = 0$ for all $k \neq 0$. ρ'_{ss} is a physical state (since we have obtained it by removing coherences from ρ_{ss}) and is a steady state as well, since it has the same elements of ρ_{ss} in the space projected by Π_0 whose evolution must be independent from the one of the elements in the space projected by Π_d. Therefore, the steady state is not unique anymore and we have proven the assertion by contradiction. ■

Proposition 3 implies the corollary that $\mathcal{L}_0$ is the only block having an eigenvalue equal to zero, while all the eigenvalues of the remaining blocks have negative real part. Another immediate consequence is the following.

Corollary 2 (Steady-state coherences). If the conditions for Proposition 1 hold and the semigroup generated by $\mathcal{L}$ is relaxing toward a unique steady state, then the only nonzero steady-state coherences in the excitation basis must have the same number of excitations in the ket and in the bra.

Proposition 3 is telling us that, when the semigroup dynamics is relaxing toward a unique steady state as it is often the case, we only need to find the eigenvalues and eigenvectors of the block $\mathcal{L}_0$ to characterize the stationary state. In particular, this restricts the range of possible steady-state coherences in which we may be interested, e.g., for thermodynamics tasks. Proposition 3 does not give information about scenarios with a broader space of steady states, such as in the presence of decoherence free subspaces and/or oscillating coherences. Further studies are needed toward this direction.

Finally, let us comment that Proposition 1 and Eq. (18) are not valid if we choose the local approach to derive the master equation [39,45,46] of a system composed of interacting subsystems (that can be rewritten as noninteracting normal modes). Indeed, the local basis used to find the jump operators would not coincide anymore with the diagonal basis of the normal modes of $\hat{H}_S$ [39,58], and this would create extra terms in the Liouvillian superoperator which would not respect the rules discussed in Sec. III B. For some particular cases, this fact may turn the global approach computationally more convenient than the local one.

IV. EXAMPLES

In this section we will propose a couple of physical examples (one for fermions, one for bosons) in which the symmetry of Eq. (18) appears, and we will show how it significantly reduces the complexity of the master equation by a block diagonalization of the Liouvillian superoperator. We choose as examples some simple low-dimensional cases, whose solution is in general already known, in order to show how to identify and employ the symmetry also in familiar scenarios. Of course, more cumbersome situations would exhibit an even more drastic dimensionality reduction. For simplicity, from now on we will drop the hat sign over the operators living in the Liouville space L.

A. Fermions

Consider a system of M noninteracting fermions, with Hamiltonian:

$$\sum_{k=1}^{M} E_k f_k^\dagger f_k. \tag{19}$$

If we let the fermions interact with local and/or collective baths through an interaction Hamiltonian H_I which satisfies one of the conditions discussed in Sec. III A, the Liouvillian superoperator will be block diagonal with each block labeled by the eigenvalues of the operator $\mathcal{N}$ in Eq. (14). We will provide the explicit form of such a Liouvillian for $M = 2$ fermions in Sec. IV A 1, being this case of utmost importance in different fields such as quantum computation or quantum thermodynamics. Before that, let us establish the dimension of each block for any M. Let us term d an (integer) eigenvalue of $\mathcal{N}$ assuming values $d = -M, \dots, -1, 0, 1, \dots, M$. The dimension of the block $\mathcal{L}_d$ is given by the number of excitation-basis vectors, written in the tensor notation of Eq. (A3), which have a difference between the number of excitations on the left and on the right of the tensor product equal to d. Taking into account all the possible combinations of suitable excitations in the vectors and all their possible permutations, the dimension of $\mathcal{L}_d$ reads

$$\dim(\mathcal{L}_d) = \sum_{k=|d|}^{M} \binom{M}{k}\binom{M}{k-|d|}. \tag{20}$$

Two interacting spins as decoupled fermions

Consider a system of two interacting spins with Hamiltonian

$$H_S = \frac{\omega_1}{2}\sigma_1^z + \frac{\omega_2}{2}\sigma_2^z + \lambda\sigma_1^x\sigma_2^x. \tag{21}$$

By employing the Jordan-Wigner transformations, a rotation and a Bogoliubov transformation (see the discussion in Appendixes C and D), we can rewrite the system Hamiltonian as

$$H_S = E_1(2f_1^\dagger f_1 - 1) + E_2(2f_2^\dagger f_2 - 1), \tag{22}$$

where f_1 and f_2 are fermionic operators satisfying the fermionic anticommutation rules: $\{f_j, f_k^\dagger\} = \delta_{jk}$, while the expressions of the energies E_1 and E_2 can be found in Eq. (D10). The interaction eigenbasis of H_S is $\{|00\rangle_f, |01\rangle_f, |10\rangle_f, |11\rangle_f\}$, and its relation with the canonical spin basis can be found in Eqs. (D17) and (D18). Although this transformation may appear redundant in the simple case of two qubits, it is fundamental for the purpose of diagonalizing more complex chains of interacting spins [53], see for instance Appendix C.

We couple each qubit to a separate thermal bath, such that the Hamiltonian of the environment is $H_E = \sum_k \Omega_k a_k^\dagger a_k + \sum_l \Omega_l' b_l^\dagger b_l$ and the interaction Hamiltonian reads

$$H_I = \sum_k g_k\sigma_1^x(a_k^\dagger + a_k) + \sum_l g_l'\sigma_2^x(b_l^\dagger + b_l), \tag{23}$$

where g_k and g_l' determine the spectral densities of the baths [1]. As mentioned before, these are not relevant for the present discussion and are assumed to display fast decaying correlation functions, inducing a Markovian evolution. We assume that the both baths are in a thermal state with temperature respectively T_1 and T_2. Such as a system is of fundamental importance, e.g., for the understanding of quantum heat transport in quantum thermodynamics [46].

Using Eqs. (D11) and (D12) we can rewrite the interaction Hamiltonian as

$$\begin{aligned} H_I = &\sum_k g_k(\cos(\theta+\phi)(f_1^\dagger + f_1) + \sin(\theta+\phi)(f_2^\dagger + f_2))(a_k^\dagger + a_k) \\ &+ \sum_l g_l'(\cos(\theta-\phi)P(f_2^\dagger - f_2) + \sin(\theta-\phi)P(f_1^\dagger - f_1))(b_l^\dagger + b_l), \end{aligned} \tag{24}$$

where P is the parity operator, and we notice that each separate bath plays now the role of a common bath between the two fermionic modes. Note that Eq. (24) satisfies the second condition on the interaction Hamiltonian presented in Sec. III A.

The interacting Hamiltonian Eq. (24) leads to the following master equation:

$$\begin{aligned} \frac{d}{dt}\rho_S(t) = &-i[H_S + H_{\rm LS}, \rho_S(t)] \\ &+ \sum_{i,j=1,2}\gamma_{ij}^\downarrow\left(f_i\rho_S(t)f_j^\dagger - \frac{1}{2}\{f_j^\dagger f_i, \rho_S(t)\}\right) \\ &+ \sum_{i,j=1,2}\gamma_{ij}^\uparrow\left(f_i^\dagger\rho_S(t)f_j - \frac{1}{2}\{f_j f_i^\dagger, \rho_S(t)\}\right) \\ &+ \sum_{i,j=1,2}\eta_{ij}^\downarrow\left(Pf_i\rho_S(t)f_j^\dagger P - \frac{1}{2}\{f_j^\dagger f_i, \rho_S(t)\}\right) \\ &+ \sum_{i,j=1,2}\eta_{ij}^\uparrow\left(f_i^\dagger P\rho_S(t)Pf_j - \frac{1}{2}\{f_j f_i^\dagger, \rho_S(t)\}\right), \end{aligned} \tag{25}$$

where the Lamb-shift Hamiltonian reads $H_{\rm LS} = \sum_{i,j=1,2}(s_{ij}^\downarrow f_j^\dagger f_i + s_{ij}^\uparrow f_j f_i^\dagger)$. The coefficients $\gamma_{ij}^\downarrow$, $\gamma_{ij}^\uparrow$, $\eta_{ij}^\downarrow$, $\eta_{ij}^\uparrow$, $s_{ij}^\downarrow$, and $s_{ij}^\uparrow$ depend on the spectral densities of the baths, on the temperature, and on the weights of each term in the interaction Hamiltonian. We do not provide their explicit value here, and we refer the interested reader to the derivation in Refs. [1,39].

We now find the Liouvillian superoperator representing the master equation (25) in the tensor product notation, as in Eq. (A5). We identify five symmetry blocks of $\mathcal{L}$, associated with the following bases: $|11\rangle_f \otimes |11\rangle_f, |10\rangle_f \otimes |10\rangle_f, |10\rangle_f \otimes |01\rangle_f, |01\rangle_f \otimes |10\rangle_f, |01\rangle_f \otimes |01\rangle_f, |00\rangle_f \otimes |00\rangle_f$ corresponding to $\mathcal{N} = 0$; $|11\rangle_f \otimes |10\rangle_f, |11\rangle_f \otimes |01\rangle_f, |10\rangle_f \otimes |00\rangle_f, |01\rangle_f \otimes |00\rangle_f$ corresponding to $\mathcal{N} = 1$; $|10\rangle_f \otimes |11\rangle_f, |01\rangle_f \otimes |11\rangle_f, |00\rangle_f \otimes |10\rangle_f, |00\rangle_f \otimes |01\rangle_f$ corresponding to $\mathcal{N} = -1$; $|11\rangle_f \otimes |00\rangle_f$ corresponding to $\mathcal{N} = 2$; $|00\rangle_f \otimes |11\rangle_f$ corresponding to $\mathcal{N} = -2$. The Liouvillian can be written as $\mathcal{L} = \bigoplus_{d=-2}^{2}\mathcal{L}_d$, where the matrices representing each block in the associated basis are

$$
\mathcal{L}_0 = \begin{pmatrix}
-\gamma_0^{\downarrow} - \eta_0^{\downarrow} & \gamma_{22}^{\uparrow} + \eta_{22}^{\uparrow} & -\gamma_{21}^{\uparrow} - \eta_{21}^{\uparrow} & -\gamma_{12}^{\uparrow} - \eta_{12}^{\uparrow} & \gamma_{11}^{\uparrow} + \eta_{11}^{\uparrow} & 0 \\
\gamma_{22}^{\downarrow} + \eta_{22}^{\downarrow} & -\xi_{11}^{\downarrow} - \xi_{22}^{\uparrow} & is_{21} - \frac{\xi_{12}^{\downarrow} - \xi_{21}^{\uparrow}}{2} & -is_{12} - \frac{\xi_{21}^{\downarrow} - \xi_{12}^{\uparrow}}{2} & 0 & \gamma_{11}^{\uparrow} + \eta_{11}^{\uparrow} \\
-\eta_{21}^{\downarrow} - \gamma_{21}^{\downarrow} & is_{12} - \frac{\xi_{21}^{\downarrow} - \xi_{12}^{\uparrow}}{2} & -i(\omega_1' - \omega_2') - \frac{\xi_0^{\downarrow} + \xi_0^{\uparrow}}{2} & 0 & -is_{12} - \frac{\xi_{21}^{\downarrow} - \xi_{12}^{\uparrow}}{2} & \gamma_{12}^{\uparrow} + \eta_{12}^{\uparrow} \\
-\eta_{12}^{\downarrow} - \gamma_{12}^{\downarrow} & -is_{21} - \frac{\xi_{12}^{\downarrow} - \xi_{21}^{\uparrow}}{2} & 0 & i(\omega_1' - \omega_2') - \frac{\xi_0^{\downarrow} + \xi_0^{\uparrow}}{2} & is_{21} - \frac{\xi_{12}^{\downarrow} - \xi_{21}^{\uparrow}}{2} & \gamma_{21}^{\uparrow} + \eta_{21}^{\uparrow} \\
\gamma_{11}^{\downarrow} + \eta_{11}^{\downarrow} & 0 & -is_{21} - \frac{\xi_{12}^{\downarrow} - \xi_{21}^{\uparrow}}{2} & is_{12} - \frac{\xi_{21}^{\downarrow} - \xi_{12}^{\uparrow}}{2} & -\xi_{22}^{\downarrow} - \xi_{11}^{\uparrow} & \gamma_{22}^{\uparrow} + \eta_{22}^{\uparrow} \\
0 & \gamma_{11}^{\downarrow} + \eta_{11}^{\downarrow} & \gamma_{12}^{\downarrow} + \eta_{12}^{\downarrow} & \gamma_{21}^{\downarrow} + \eta_{21}^{\downarrow} & \gamma_{22}^{\downarrow} + \eta_{22}^{\downarrow} & -\gamma_0^{\uparrow} - \eta_0^{\uparrow}
\end{pmatrix}, \quad (26)
$$

$$
\mathcal{L}_1 = \begin{pmatrix}
-i\omega_2' - \xi_{11}^{\downarrow} - \frac{\xi_{22}^{\downarrow} + \xi_{22}^{\uparrow}}{2} & is_{21} - \frac{\xi_{12}^{\downarrow} - \xi_{21}^{\uparrow}}{2} & \eta_{21}^{\uparrow} - \gamma_{21}^{\uparrow} & \gamma_{11}^{\uparrow} - \eta_{11}^{\uparrow} \\
is_{12} - \frac{\xi_{21}^{\downarrow} - \xi_{12}^{\uparrow}}{2} & -i\omega_1' - \xi_{22}^{\downarrow} - \frac{\xi_{11}^{\downarrow} + \xi_{11}^{\uparrow}}{2} & \eta_{22}^{\uparrow} - \gamma_{22}^{\uparrow} & \gamma_{12}^{\uparrow} - \eta_{12}^{\uparrow} \\
\eta_{21}^{\downarrow} - \gamma_{21}^{\downarrow} & \eta_{22}^{\downarrow} - \gamma_{22}^{\downarrow} & -i\omega_1' - \xi_{22}^{\uparrow} - \frac{\xi_{11}^{\downarrow} + \xi_{11}^{\uparrow}}{2} & -is_{12} - \frac{\xi_{21}^{\downarrow} - \xi_{12}^{\uparrow}}{2} \\
\gamma_{11}^{\downarrow} - \eta_{11}^{\downarrow} & \gamma_{12}^{\downarrow} - \eta_{12}^{\downarrow} & -is_{21} - \frac{\xi_{12}^{\downarrow} - \xi_{21}^{\uparrow}}{2} & -i\omega_2' - \xi_{11}^{\uparrow} - \frac{\xi_{22}^{\downarrow} + \xi_{22}^{\uparrow}}{2}
\end{pmatrix}, \quad (27)
$$

$\mathcal{L}_{-1} = \mathcal{L}_1^*$, $\mathcal{L}_2 = -i(\omega_1' + \omega_2') - \xi_0^{\downarrow} - \xi_0^{\uparrow}$ and $\mathcal{L}_{-2} = \mathcal{L}_2^*$. When convenient, we have used the abbreviations $\omega_1' = 2E_1 + s_{11}^{\downarrow} - s_{11}^{\uparrow}$, $\omega_2' = 2E_2 + s_{22}^{\downarrow} - s_{22}^{\uparrow}$, $s_{ij} = s_{ij}^{\downarrow} - s_{ji}^{\uparrow}$, $\gamma_0^{\downarrow\uparrow} = \gamma_{11}^{\downarrow\uparrow} + \gamma_{22}^{\downarrow\uparrow}$, $\eta_0^{\downarrow\uparrow} = \eta_{11}^{\downarrow\uparrow} + \eta_{22}^{\downarrow\uparrow}$, $\xi_{ij}^{\downarrow\uparrow} = \gamma_{ij}^{\downarrow\uparrow} + \eta_{ij}^{\downarrow\uparrow}$, and $\xi_0^{\downarrow\uparrow} = \gamma_0^{\downarrow\uparrow} + \eta_0^{\downarrow\uparrow}$.

Note that assuming a local master equation instead of Eq. (25) would lead to extra terms connecting, for instance, the block $\mathcal{L}_0$ with the blocks $\mathcal{L}_{\pm 2}$ [39]. Therefore, the block decomposition would not be valid in this case.

A very similar structure was found for the Liouvillian of two uncoupled spins in a common bath [57], where the block separation was exploited to find the analytical eigenvalues describing the decay of the system. We thus understand the help brought by the symmetry in Eq. (18) to the present example: instead of having to find the eigenvalues and eigenvectors of a 16×16 matrix, we restrict ourselves to the analysis of a 6×6 and a 4×4 matrix. Figure 1 depicts how the elements of the density matrix of the system written in the excitation basis appear in separate blocks of the master equation (each color representing an independent block).

Furthermore, if we are interested in finding the steady state of the evolution and the latter is unique, we just have to analyze the matrix $\mathcal{L}_0$. To be sure that the condition on the uniqueness holds, one has to check that no decoherence-free subspaces are present. Their appearance can be detected *a priori* using different conditions on the interaction

$$
\rho_S = \begin{pmatrix}
\rho_{11,11} & \rho_{11,10} & \rho_{11,01} & \rho_{11,00} \\
\rho_{10,11} & \rho_{10,10} & \rho_{10,01} & \rho_{10,00} \\
\rho_{01,11} & \rho_{01,10} & \rho_{01,01} & \rho_{01,00} \\
\rho_{00,11} & \rho_{00,10} & \rho_{00,01} & \rho_{00,00}
\end{pmatrix}
$$

FIG. 1. Density matrix of the state of the system with Hamiltonian equation (22) in the fermionic interactions basis. The master equation driven by the Liouvillian $\mathcal{L}$ couples only elements of the density matrix with the same color. In particular, the elements of the block $\mathcal{L}_0$ are represented by the color red, of $\mathcal{L}_1$ by the color green, of $\mathcal{L}_{-1}$ by the color blue, of $\mathcal{L}_2$ by the color purple, and of $\mathcal{L}_{-2}$ by the color orange.

Hamiltonian or on the master equation [50], otherwise they can be revealed by the presence of more than one null eigenvalue in the spectrum of the Liouvillian superoperator. Since we have set nonzero, unbalanced temperatures of the baths, the steady state may contain coherences as well, but only the ones corresponding to the eigenvalue 0 of $\mathcal{N}$, namely $\rho_{10,01}$ and $\rho_{01,10}$. The same steady-state coherences were found using a nonsecular master equation in a couple of recent works [22,59]. We will provide an example of the appearance of these coherences below and in the next example about harmonic oscillators.

Note that, if we had performed the full secular approximation instead of the partial one, we would have introduced a broader symmetry on the superoperator level, dividing the block $\mathcal{L}_0$ into two additional parts. Indeed, if the spectrum of H_S is nondegenerate, the full secular approximation decouples coherences and populations [1]. The symmetry generated by $\mathcal{N}$ is therefore providing us with new "selection rules" that indicate the allowed transitions between elements of the density matrix: in the partial secular regime some of the coherences may exchange "amplitude" with the diagonal elements. We can visualize this through a concrete case of the two-coupled-qubits example: let us consider a scenario with $\omega_1 = 1$, $\omega_2 = 1$, $\lambda = 0.01$, $T_1 = \omega_1/k_B$, $T_2 = \omega_1/10k_B$, and Ohmic spectral densities (from now on for simplicity we use dimensionless units for time and energy). Using these values, the fermionic energies read $2E_1 = 1.01005$ and $2E_2 = 0.99005$. μ denotes the strength of the qubit-bath coupling, and considering the weak-coupling limit we set $\mu = 10^{-1.5}$. According to Eq. (9), $\tau_R \approx 1000$ and therefore the partial secular approximation must conserve the terms in the master equation associated with the frequency difference $2E_1 - 2E_2 = 0.02$, which does not satisfy the condition in Eq. (7). Using the above values, we can calculate the coefficients of the master equation (25) according to the discussion in Ref. [1] and we can compute the dynamics of the two qubits. According to the suitable conditions [50], we have checked that no decoherence-free subspace is present in this scenario.

We now want to visualize how the partial secular approximation induces selection rules between different elements of the density matrix: we consider the evolution of the two

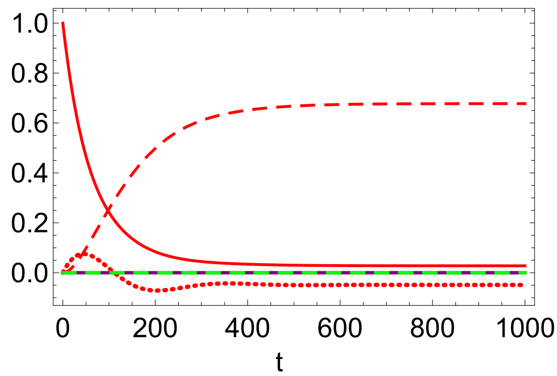

FIG. 2. Mean value of different two-qubit observables as a function of time, when the evolution starts in the state $|11\rangle_f$ and we use the master equation (25) in partial secular approximation. As defined in the main text, we plot $P_{11}(t)$ (solid red), $P_{00}(t)$ (dashed red), $C_0(t)$ (dotted red), $C_1(t)$ (dashed green), and $C_2(t)$ (solid purple). C_1 and C_2 remain null during the evolution, while using the master equation in partial secular approximation C_0 varies and stabilizes to a nonzero value after the thermalization time, showing the appearance of steady-state coherences. On the contrary, the full secular approximation would keep C_0 null as well. The units are dimensionless.

qubits starting from the excited fermionic state $|11\rangle_f$, i.e., $\rho_S(0) = |11\rangle_f\langle 11|$, whose dynamics is driven by the block $\mathcal{L}_0$. We monitor the expectation value of some observables which pertain to different blocks of the Liouvillian superoperator as a function of time, in particular we choose:

(i) $P_{11}(t) = \mathrm{Tr}[\rho_S(t)|11\rangle_f\langle 11|] = \rho_{11,11}(t)$,
(ii) $P_{00}(t) = \mathrm{Tr}[\rho_S(t)|00\rangle_f\langle 00|] = \rho_{00,00}(t)$,
(iii) $C_0(t) = \mathrm{Tr}[\rho_S(t)(f_1^\dagger f_2 + f_2^\dagger f_1)] = 2\,\mathrm{Re}[\rho_{01,10}(t)]$,
(iv) $C_1(t) = \mathrm{Tr}[\rho_S(t)(f_1 + f_1^\dagger)] = 2\,\mathrm{Re}[\rho_{11,01}(t)] + 2\,\mathrm{Re}[\rho_{10,00}(t)]$,
(v) $C_2(t) = \mathrm{Tr}[\rho_S(t)(f_1^\dagger f_2^\dagger + f_2 f_1)] = 2\,\mathrm{Re}[\rho_{11,00}(t)]$.

P_{11}, P_{00}, and C_0 depend on elements of the block $\mathcal{L}_0$, while C_1 of the block $\mathcal{L}_1$ and C_2 of the block $\mathcal{L}_2$. Figure 2 depicts their evolution: P_{11} is the only nonzero mean value at time 0. Therefore, the symmetry brought by the partial secular approximation $[\mathcal{N}, \mathcal{L}] = 0$ denies the possibility that C_1 and C_2 may change their value during the evolution, since their dynamics is driven by blocks different from $\mathcal{L}_0$. On the contrary, C_0 increases and stabilizes to a nonzero value at infinite time, since it is the mean value of the observable expressing the exchange of excitations between the fermions, whose dynamics is driven by $\mathcal{L}_0$.

Let us now briefly discuss how things would change if we applied the full secular approximation to derive the master equation (25), i.e., if we removed the terms with $i \neq j$. The full secular approximation decouples coherences and populations [1], therefore, in the scenario discussed before, not only would it inhibit any transition that may "activate" C_1 and C_2, but it would also keep C_0 null, given that the latter depends on the density matrix element $\rho_{01,10}$. This means that, in Fig. 2, the full secular approximation would make the dotted red line (C_0) overlap with the green and purple lines (C_1 and C_2), thus proving itself not suitable to treat the current scenario [39].

B. Bosons

If we consider a generic bosonic system for which Eq. (18) holds, we will still have a block diagonalization of the Liouvillian superoperator which will simplify the resolution of the master equation, but each block will have infinite dimension. Here we want to focus on a simpler case in which the symmetry expressed by Eq. (18) leads to a dimensionality reduction as well: we restrict ourselves to the space of Gaussian states [60] and we consider only a master equation conserving Gaussianity. Therefore, we only need to analyze the dynamics of the covariance matrix, neglecting any displacement which may be eliminated through a suitable transformation.

Let us consider a system of M noninteracting bosons with Hamiltonian:

$$H_S = \sum_{k=1}^{M} E_k a_k^\dagger a_k. \tag{28}$$

Given the presence of local or common baths leading to a Gaussian Markovian master equation, we want to study the dynamics of a Gaussian state with no displacement. For convenience, we choose to write the covariance matrix of the state using the creation and annihilation operators, i.e., a generic element of the covariance matrix may be written in one of these three forms:

$$\langle a_i^\dagger a_j^\dagger\rangle \quad \text{or} \quad \langle a_i^\dagger a_j\rangle \quad \text{or} \quad \langle a_i a_j\rangle, \tag{29}$$

where the average is performed on the chosen Gaussian state. We define as δ the difference between number of creations and number of annihilations in an element of the covariance matrix Eq. (29), assuming values 2, 0, -2, respectively.

It is easy to understand what the symmetry defined by Eq. (18) is telling us about the evolution of the covariance matrix: the dynamics of an element of the covariance matrix with value δ can only be a function of elements of the covariance matrix with the same value δ.[3] We can collect the elements of the covariance matrix Eq. (29) (which cannot be trivially obtained through commutations of the other elements) in a vector $\mathbf{x}$. The evolution of $\mathbf{x}$ as a function of time is then given by the formula

$$\frac{d\mathbf{x}}{dt} = B\mathbf{x} + \mathbf{b}. \tag{30}$$

The matrix B is block diagonalized labeling each block with the value δ: $B = \bigoplus_{\delta=-2,0,2} B_\delta$. Furthermore, $\langle a_i^\dagger a_j^\dagger\rangle = \langle a_i a_j\rangle^*$ and the symmetry assures us that these two moments do not couple in the master equation, therefore the block B_2 is

[3]This property can be extended to non-Gaussian states, where the nth moments must be taken into account: the master equation describing the evolution of the nth moment $\langle \underbrace{a_i^\dagger a_j^\dagger \ldots}_{l\text{ creation}} \underbrace{\ldots a_r a_s}_{n-l\text{ annihilations}}\rangle$ with $\delta = 2l - n$ can only be a function of mth moments with the same value of δ (difference between number of creations and number of annihilations in the moment).

trivially obtained by the block B_{-2}. We can now calculate the dimension of each block B_δ:

$$\dim(B_0) = M^2,\qquad \dim(B_{\pm 2}) = \binom{M+2-1}{2}. \tag{31}$$

Two bosons in a common bath

As an example we consider the system of two displaced noninteracting bosons with Hamiltonian:

$$H_S = \sum_{k=1,2} (\omega_k a_k^\dagger a_k - \alpha_k a_k - \alpha_k^* a_k^\dagger). \tag{32}$$

The Hamiltonian can be recast in the standard form of Eq. (16) through a suitable displacement operator $D(\boldsymbol{\alpha})$ [60]: $D(\boldsymbol{\alpha})^\dagger a_k D(\boldsymbol{\alpha}) = a_k + \alpha_k$. Therefore we have

$$H_S = \sum_{k=1,2} E_k a_k^\dagger a_k, \tag{33}$$

which describes two noninteracting harmonic oscillators. We couple the system to a common bosonic environment $H_E = \sum_l \Omega_l c_l^\dagger c_l$ in a thermal state with temperature $T > 0$. The system-bath interaction Hamiltonian is

$$H_I = \sum_l g_l (a_1 + a_1^\dagger + a_2 + a_2^\dagger)(c_l + c_l^\dagger), \tag{34}$$

where g_l determines the spectral density, which is not relevant for the present discussion. The evolution of the system coupled to the environment is given by the master equation with Liouvillian:

$$\mathcal{L}^\dagger[O] = i[H_S + H_{\rm LS}, O] + \sum_{ij=1,2} \gamma_{ij}^\downarrow \left(a_i^\dagger O a_j - \frac{1}{2}\{a_i^\dagger a_j, O\}\right) + \sum_{ij=1,2} \gamma_{ij}^\uparrow \left(a_i O a_j^\dagger - \frac{1}{2}\{a_i a_j^\dagger, O\}\right), \tag{35}$$

where O is an operator acting on the Hilbert space of the system, and $\gamma_{ij}^\downarrow$ and $\gamma_{ij}^\uparrow$ are, respectively, the coefficients describing the decay and the absorption, which depend on the spectral density and on the temperature of the environment [1]. The Lamb-shift Hamiltonian reads

$$H_{\rm LS} = \sum_{ij=1,2} s_{ij} a_i^\dagger a_j. \tag{36}$$

The elements γ_{12} and γ_{21} are different from zero only if the harmonic oscillators are slightly detuned (or not detuned at all) [39]. We remind that, assuming that the initial state is Gaussian, then it will remain Gaussian due to the form of Eq. (35).

The relevant elements of the covariance matrix can be collected in a vector $\mathbf{x}$ of dimension 10. In particular, we choose to parametrize it according to the basis $\langle a_1^\dagger a_1^\dagger\rangle$, $\langle a_2^\dagger a_2^\dagger\rangle$, $\langle a_1^\dagger a_2^\dagger\rangle$ with $\delta = 2$. $\langle a_1 a_1\rangle$, $\langle a_2 a_2\rangle$, $\langle a_1 a_2\rangle$ with $\delta = -2$. $\langle a_1^\dagger a_1\rangle$, $\langle a_2^\dagger a_2\rangle$, $\langle a_1^\dagger a_2\rangle$, $\langle a_2^\dagger a_1\rangle$ with $\delta = 0$. The master equation describing the evolution of $\mathbf{x}$ has the form of Eq. (30). The vector $\mathbf{b}$ can be written as $\mathbf{b} = \oplus_{\delta=-2,0,2}\mathbf{b}_\delta$. We have that $\mathbf{b}_{\pm 2} = \mathbf{0}$, while

$$\mathbf{b}_0 = \begin{pmatrix} \gamma_{11}^\uparrow \\ \gamma_{22}^\uparrow \\ \gamma_{12}^\uparrow \\ \gamma_{21}^\uparrow \end{pmatrix}. \tag{37}$$

The matrix B describes how the elements of the covariance matrix are coupled together in the master equation, and it is block diagonal according to $B = \bigoplus_{\delta=-2,0,2} B_\delta$. The blocks are given by

$$B_0 = \begin{pmatrix} -\gamma_1^b & 0 & \frac{-2is_{12}-\gamma_{12}^\downarrow+\gamma_{21}^\uparrow}{2} & \frac{2is_{21}-\gamma_{21}^\downarrow+\gamma_{12}^\uparrow}{2} \\ 0 & -\gamma_2^b & \frac{2is_{12}-\gamma_{12}^\downarrow+\gamma_{21}^\uparrow}{2} & \frac{-2is_{21}-\gamma_{21}^\downarrow+\gamma_{12}^\uparrow}{2} \\ \frac{-2is_{21}-\gamma_{21}^\downarrow+\gamma_{12}^\uparrow}{2} & \frac{2is_{21}-\gamma_{21}^\downarrow+\gamma_{12}^\uparrow}{2} & i\Delta\omega - \frac{\gamma_1^b+\gamma_2^b}{2} & 0 \\ \frac{2is_{12}-\gamma_{12}^\downarrow+\gamma_{21}^\uparrow}{2} & \frac{-2is_{12}-\gamma_{12}^\downarrow+\gamma_{21}^\uparrow}{2} & 0 & -i\Delta\omega - \frac{\gamma_1^b+\gamma_2^b}{2} \end{pmatrix}, \tag{38}$$

$$B_{-2} = \begin{pmatrix} -2iE_1' - \gamma_1^b & -2is_{12} - \gamma_{12}^\downarrow + \gamma_{21}^\uparrow & 0 \\ -is_{21} - \frac{\gamma_{21}^\downarrow-\gamma_{12}^\uparrow}{2} & -i(E_1'+E_2') - \frac{\gamma_1^b+\gamma_2^b}{2} & -is_{12} - \frac{\gamma_{12}^\downarrow-\gamma_{21}^\uparrow}{2} \\ 0 & -2is_{21} - \gamma_{21}^\downarrow + \gamma_{12}^\uparrow & -2iE_2' - \gamma_2^b \end{pmatrix}, \tag{39}$$

and $B_2 = B_{-2}^*$. We have defined $E_1' = E_1 + s_{11}$, $E_2' = E_2 + s_{22}$, $\Delta\omega = E_1' - E_2'$, $\gamma_j^b = \gamma_{jj}^\downarrow - \gamma_{jj}^\uparrow$. To find the steady state of the system we have to solve the equation $B\mathbf{x}_{ss} + \mathbf{b} = \mathbf{0}$. Therefore, the elements of the covariance matrix with $\delta \neq 0$ vanish in the steady state. On the contrary, in the case in which the harmonic oscillators are slightly detuned and $\gamma_{12} \neq 0$, all the elements with $\delta = 0$ have a nonzero component for $t \to \infty$, and in particular $\langle a_1^\dagger a_2\rangle_{ss}$ and $\langle a_2^\dagger a_1\rangle_{ss}$ do not vanish, i.e., we observe steady-state coherences. The analytical form of the steady state can be obtained by solving the system of four differential equations given by $B_0\mathbf{x}_{ss}^{(\delta=0)} + \mathbf{b}_0 = 0$.

V. DISCUSSION AND CONCLUSIONS

In this paper we have shown how the Liouvillian superoperator $\mathcal{L}$ of a broad class of open quantum systems can be block diagonalized through a symmetry on the superoperator level, namely the invariance under the action of the number superoperator $\mathcal{N}$, defined in Eq. (14), such that $[\mathcal{N}, \mathcal{L}] = 0$. This symmetry arises when we derive the standard Bloch-Redfield master equation of the open system applying a suitable partial secular approximation whose condition is given by Eq. (7). The requirements for the microscopic model are that the system Hamiltonian can be recast as M noninteracting bosonic or fermionic modes [Eq. (16)] and that the system operators in the interaction Hamiltonian satisfy the conditions discussed at the end of Sec. III A, which are usually fulfilled in the majority of physical systems of importance to quantum information or condensed matter physics. This includes, for instance, any system with Hamiltonian quadratic in the bosonic or fermionic operators, and coupled to a thermal bath through operators which are linear in the field operators, as well as some spin systems.

The existence of the symmetry is formalized and proven in Proposition 1. Corollary 1 states that such symmetry implies the invariance under the action of the parity superoperator as well. Proposition 2 shows that we can exploit Proposition 1 to decompose the Liouvillian superoperator into blocks, and that in the fermionic case only $M + 1$ of them are independent. This greatly reduces the complexity of the master equation. Furthermore, each block may be the only part of the Liouvillian we have to manipulate in order to find a certain physical quantity, for example Proposition 3 shows that, when unique, the steady state is determined only by one single block. This implies that the allowed steady-state coherences in the excitation basis of an unique steady state are only the ones with equal number of excitations in the ket and the bra, as formalized in Corollary 2.

A couple of examples are also discussed. In Sec. IV A we have found the dimension of each block $\mathcal{L}_d$ of the Liouvillian superoperator in the case of a system of M fermionic modes [Eq. (20)], and we have shown how to apply this to a system of two coupled qubits. In this scenario, an originally 16×16 Liouvillian is decomposed into five blocks of dimension 6, 4, 4, 1, and 1. The information about the steady state is contained in the 6×6 block only. The decomposition greatly simplifies the master equation and also allows us to obtain some analytical solutions. Then, in Sec. IV B we have discussed the case of bosons, focusing in particular on Gaussian states. We have shown how to decompose the equation for the evolution of the covariance matrix employing the symmetry of the number superoperator, and we have applied it to study the case of two harmonic oscillators in a common bath. In the presence of small detuning, we have detected steady-state coherences by focusing on a system of only four linear equations, instead of the original system of ten equations.

These results may be relevant in disparate fields. For instance, reducing the complexity of the master equation describing transport in quantum systems is of great importance [61], and our discussion may be especially relevant for materials which exhibit *quasidegeneracies* in the Hamiltonian spectrum and thus require a master equation in partial secular approximation [62]. The latter is also important to study the heat current from two unbalanced reservoirs, since it solves any deficiency that a global master equation may display with respect to a local one [39]. The symmetry generated by $\mathcal{N}$ may be also relevant in the field of quantum metrology. Indeed, as discussed in Sec. III B it may be seen as a generalization of the concept of phase-covariant master equation, which plays a fundamental role in defining the limits for the frequency estimation of a single qubit [54,63–65]. Therefore, a protocol for the frequency estimation of multiple detuned qubits should rely on our result to distinguish between the possible noise models and their origin. Finally, Proposition 3 and Corollary 2 are very relevant in quantum thermodynamics and quantum thermalization. Indeed, they define a strict law on the possible steady-state coherences that may appear in the steady state of a Markovian process. The relation between coherences and diagonal elements is also important to improve the performance of quantum thermal machines [66].

Possible extensions of this work could address other situations where the number superoperator symmetry can arise. In particular, beyond stationary environments considered here, nonstationary autocorrelation functions of the bath would add a temporal dependence to the coefficients of the Lamb-shift Hamiltonian and of the dissipator in Eqs. (5) and (6). This would affect the way in which we perform the partial secular approximation. As a consequence, there may exist scenarios in which the symmetry is broken. Consider for instance a single-mode electromagnetic field in a squeezed bath [1]: the master equation would contain terms of the form $a\rho_S a$, where a is the annihilation operator of the field. Clearly, in this case $[\mathcal{N}, \mathcal{L}] \neq 0$. Note however that we would still recover the symmetry of the parity superoperator $[\mathcal{P}, \mathcal{L}] = 0$. Different scenarios may arise considering different states of the environment, and further investigation is needed to extend our work to these cases.

A further direction could be exploring nonlinear scenarios beyond quadratic system Hamiltonians, even if the latter include many bosonic and fermionic systems of interest to quantum information. In particular, for systems of many coupled spins where the number of spin excitations is not conserved, even if diagonalization through the Jordan-Wigner transformations is possible, the resulting fermionic Hamiltonian generally depends on a collective phase, violating the "noninteracting" condition. In these scenarios, the validity of the symmetry $[\mathcal{N}, \mathcal{L}] = 0$ must be checked case by case, using the physical considerations discussed in Sec. III. On the contrary, the block decomposition holds for any excitation-preserving system of spins in common or separate thermal baths (with a final requirement on the interaction Hamiltonian).

The extension of Proposition 3 to scenarios with more than one steady state, e.g., in the presence of decoherence free subspaces or oscillating coherences, would also be interesting. In particular, some open questions not addressed here are: does the block $\mathcal{L}_0$ contain all the information about any steady state of the system? If not, are there particular cases in which this holds? Can we find an analogous theorem for oscillating coherences? Investigation about the same symmetry for non-Markovian master equations in the weak coupling limit may be interesting as well. In particular, we expect to find the same results for the case of a time-local non-Markovian master equation in the *secular regime* [67], while nonsecular terms would break the symmetry. Finally, it would be useful to employ our findings to implement a fast, manageable code to solve the dynamics of the open system by exploit-ing its symmetry, as already done for the case of identical atoms [29].

ACKNOWLEDGMENTS

M.C. acknowledges interesting discussions with Bassano Vacchini, Bruno Bellomo, Giacomo Guarnieri, and Gerhard Dorn, and thanks Salvatore Lorenzo for useful hints. The authors acknowledge funding from MINECO/AEI/FEDER through projects EPheQuCS FIS2016-78010-P, the María de Maeztu Program for Units of Excellence in R&D (MDM-2017-0711), and the CAIB postdoctoral program, support from CSIC Research Platform PTI-001 and partial funding of M.C. from Fondazione Angelo della Riccia.

APPENDIX A: THE FORMALISM OF GKLS MASTER EQUATIONS

1. From the Bloch-Redfield to the Lindblad equation

The fact that, in general, the Bloch-Redfield master equation does not preserve positivity and is not in the GKLS form (or Lindblad form) [7,8] is a very well-known issue [68]. The standard procedure to derive a Markovian master equation makes use of the full secular approximation [1,3], i.e., removes all the terms with $\omega \neq \omega'$ in Eqs. (5) and (6), in order to recover the semigroup structure of a master equation in the Lindblad form. This, however, may lead to major mistakes when the condition in Eq. (7) is not fulfilled [39]. Nonetheless, some recent studies have shown that the PSA performed through a suitable coarse graining does lead to a GKLS master equation [40,41], as can be also found in a previous work which did not mention the PSA [69]. This method of applying the PSA is analogous to the one used in the present paper, based on the condition in Eq. (7), up to a negligible error. A related discussion is provided in Ref. [43]. As a matter of fact, the Bloch-Redfield master equation does follow the dynamics of a GKLS master equation up to an error due to the approximation of the dynamics of the microscopic model to a Markovian evolution. A significant deviation of the Bloch-Redfield master equation from the Lindblad form must be considered as a signature of the failure of the Born-Markov approximations to describe the physical model, and not vice versa, as proven in Ref. [42].

For the reasons explained above, we are allowed to assume that the master equation in PSA with Liouvillian Eq. (4) can be rewritten in the GKLS or Lindblad form as in Eq. (10). The Lindblad operators become linear combinations of the jump operators $\hat{A}_\alpha$, and can be obtained for each specific case by diagonalizing the matrix $\gamma_{\alpha\beta}(\omega,\omega')$ in Eq. (6) [40,41]. Analogously, we can write the master equation in the Lindblad form in the Heisenberg picture [1]:

$$\frac{d}{dt}\hat{J}(t) = i[\hat{H}', \hat{J}(t)] + \sum_{l=1}^{N^2-1} \hat{F}_l^\dagger \hat{J}(t)\hat{F}_l - \frac{1}{2}\{\hat{F}_l^\dagger \hat{F}_l, J(t)\}, \tag{A1}$$

where $\hat{J} = \hat{J}^\dagger$ is an observable living in L, whose expectation value can be found as $\langle \hat{J}(t)\rangle = \mathrm{Tr}[\hat{J}(t)\rho_S] = \mathrm{Tr}[\hat{J}\rho_S(t)]$.

2. Working with superoperators

It is very convenient to extend the bra-ket notation to the Liouville space L [27,57]. Suppose that $\{|e_j\rangle\}_{j=1}^N$ is a basis of the Hilbert space H_S. Then any operator $\hat{O}$ (or equivalently density matrix) in L can be written as

$$\hat{O} = \sum_{j,k=1}^{N} O_{jk}|e_j\rangle\langle e_k|. \tag{A2}$$

We now perform the following isomorphism, passing from a description of $\hat{O}$ as an operator acting on H_S to a description as a N^2-dimensional vector:

$$\hat{O} \to |O\rangle\rangle = \sum_{j,k=1}^{N} O_{jk}|e_j\rangle \otimes |e_k\rangle. \tag{A3}$$

Given $\hat{O}, \hat{R} \in \mathsf{L}$, the reader can verify that this N^2-dimensional space is furnished with the Hilbert-Schmidt scalar product $\langle\langle O|R\rangle\rangle = \mathrm{Tr}(\hat{O}^\dagger \hat{R})$, and that the following properties hold:

$$|OR\rangle\rangle = \hat{O}\otimes \mathbb{I}_N|R\rangle\rangle, \quad |RO\rangle\rangle = \mathbb{I}_N \otimes \hat{O}^T|R\rangle\rangle, \tag{A4}$$

where $\mathbb{I}_N$ is the $N \times N$ identity matrix.

Using Eq. (A4), we can now write the explicit form of the Liouvillian superoperator starting from the Bloch-Redfield master equation in Eqs. (3), (5), and (6):

$$\mathcal{L} = -i((\hat{H}_S + \hat{H}_{\mathrm{LS}})\otimes \mathbb{I}_N - \mathbb{I}_N \otimes (\hat{H}_S + \hat{H}_{\mathrm{LS}})^T) + \sum_{\alpha,\beta}\sum_{(\omega,\omega')\in \mathsf{PSA}} \gamma_{\alpha\beta}(\omega,\omega')\Big(\hat{A}_\beta(\omega)\otimes \hat{A}_\alpha^*(\omega') - \frac{1}{2}\{\hat{A}_\alpha^\dagger(\omega')\hat{A}_\beta(\omega)\otimes \mathbb{I}_N + \mathbb{I}_N \otimes [\hat{A}_\alpha^\dagger(\omega')\hat{A}_\beta(\omega)]^T\}\Big). \tag{A5}$$

APPENDIX B: PROOF OF PROPOSITION 1

We want to prove that $[\mathcal{N}, \mathcal{L}] = 0$. For convenience we work using the isomorphism "flattening" matrices into vectors [see Appendix A 2, Eq. (A3)], so that $\mathcal{L}$ can be written as in Eq. (A5) and $\mathcal{N}$ as in Eq. (15). Looking at the structure of $\mathcal{L}$, we recognize four different parts of the Liouvillian that must commute with $\mathcal{N}$; in particular, to proof the statement it is sufficient to verify the following four assertions:

(1) $[\mathcal{N}, \hat{H}_S \otimes \mathbb{I}_N] = [\mathcal{N}, \mathbb{I}_N \otimes \hat{H}_S^T] = 0$.
(2) $[\mathcal{N}, \hat{A}_\beta(\omega)\otimes \hat{A}_\alpha^*(\omega')] = 0$ for all α, β and $(\omega,\omega') \in$ PSA.
(3) $[\mathcal{N}, \hat{A}_\alpha^\dagger(\omega')\hat{A}_\beta(\omega)\otimes \mathbb{I}_N] = 0$ for all α, β and $(\omega,\omega') \in$ PSA.
(4) $[\mathcal{N}, \mathbb{I}_N \otimes (\hat{A}_\alpha^\dagger(\omega')\hat{A}_\beta(\omega))^T] = 0$ for all α, β and $(\omega,\omega') \in$ PSA.

This means that the value of the coefficients of the master equation does not play a role in the appearance of the symmetry.

Assertion (1) is easily proven: the system Hamiltonian Eq. (16) cannot change the number of particles in any mode, since $[\hat{H}_S, \hat{n}_k] = 0\ \forall k$, and thus $[\hat{H}_S, \hat{N}] = 0$, therefore $[\mathcal{N}, \hat{H}_S \otimes \mathbb{I}_N] = 0$.

Given the Hamiltonian of a system of M modes, $\hat{H}_S = \sum_{k=1}^M E_k \hat{n}_k$, we write an eigenvector as $|e\rangle$, with $\hat{H}_S|e\rangle = e|e\rangle$ and $e = \sum_{k=1}^M E_k n_k^e$, where n_k^e is the number of excitation in each mode of $|e\rangle = |n_1^e, \ldots, n_M^e\rangle$. The total number of particles in $|e\rangle$ is given by $n^e = \sum_{k=1}^M n_k^e$. Using the same notation for generic eigenvectors $|e'\rangle, |\epsilon\rangle, |\epsilon'\rangle$, we write the jump operators as $\hat{A}_\beta(\omega) = \sum_{e'-e=\omega} |e\rangle\langle e|\hat{A}_\beta|e'\rangle\langle e'|$, $\hat{A}_\alpha(\omega') = \sum_{\epsilon'-\epsilon=\omega'} |\epsilon\rangle\langle\epsilon|\hat{A}_\alpha|\epsilon'\rangle\langle\epsilon'|$. Let us now consider Assertion (2): we write the commutator as

$$\begin{aligned}
&[\mathcal{N}, \hat{A}_\beta(\omega)\otimes\hat{A}_\alpha^*(\omega')] \\
&\quad= \hat{N}\hat{A}_\beta(\omega)\otimes\hat{A}_\alpha^*(\omega') - \hat{A}_\beta(\omega)\hat{N}\otimes\hat{A}_\alpha^*(\omega') \\
&\qquad+\hat{A}_\beta(\omega)\otimes\hat{A}_\alpha^*(\omega')\hat{N}^T - \hat{A}_\beta(\omega)\otimes\hat{N}^T\hat{A}_\alpha^*(\omega') \\
&\quad= \sum_{e'-e=\omega}(n^e - n^{e'})|e\rangle\langle e|\hat{A}_\beta|e'\rangle\langle e'|\otimes\hat{A}_\alpha^*(\omega') \\
&\qquad-\hat{A}_\beta(\omega)\otimes\sum_{\epsilon'-\epsilon=\omega'}(n^\epsilon - n^{\epsilon'})|\epsilon\rangle\langle\epsilon|\hat{A}_\alpha^*|\epsilon'\rangle\langle\epsilon'|. \quad \text{(B1)}
\end{aligned}$$

Since $(\omega,\omega')\in\mathsf{PSA}$, according to Eq. (7) we must have $\omega-\omega' = \mathcal{O}_{t^*}(\mu^2)$, therefore $\sum_{k=1}^M E_k(n_k^{e'} - n_k^e - n_k^{\epsilon'} + n_k^\epsilon) = \mathcal{O}_{t^*}(\mu^2)$ or $\sum_{k=1}^M E_k(n_k^{e'} + n_k^\epsilon) = \sum_{k=1}^M E_k(n_k^e + n_k^{\epsilon'}) + \mathcal{O}_{t^*}(\mu^2)$. But, assuming *condition II* on the interaction Hamiltonian defined at the end of Sec. III A (which comprises *condition I* as well), the last line means that $\sum_{k=1}^M (n_k^{e'} + n_k^\epsilon) = \sum_{k=1}^M (n_k^e + n_k^{\epsilon'})$, that is to say, $(n^e - n^{e'}) = (n^\epsilon - n^{\epsilon'})$, for any couple of $|e\rangle, |e'\rangle$ or $|\epsilon\rangle, |\epsilon'\rangle$ in Eq. (B1). Therefore, the commutator in Eq. (B1) vanishes and we have proven Assertion (2). This proof shows us how we can relax *condition II* on the interaction Hamiltonian: it is sufficient to assume it only on the energies which enter in the expression of each possible $(\omega,\omega')\in\mathsf{PSA}$. For instance, suppose we have a system of two modes and all the $\hat{A}_\alpha$ are second-degree polynomials in the creation and annihilation operators of the modes. Then we just need to require that $2E_1 \neq E_2 + \mathcal{O}_{t^*}(\mu^2)$ or vice versa, in order to eliminate all the "unbalanced" terms through the partial secular approximation.

Next, we consider Assertion (3):

$$\begin{aligned}
&[\mathcal{N}, \hat{A}_\alpha^\dagger(\omega')\hat{A}_\beta(\omega)\otimes\mathbb{I}_N] \\
&\quad= \hat{N}\hat{A}_\alpha^\dagger(\omega')\hat{A}_\beta(\omega)\otimes\mathbb{I}_N - \hat{A}_\alpha^\dagger(\omega')\hat{A}_\beta(\omega)\hat{N}\otimes\mathbb{I}_N \\
&\quad= \sum_{\substack{\epsilon-\epsilon'=\omega' \\ e-\epsilon'=\omega}}(n^\epsilon - n^e)|\epsilon\rangle\langle\epsilon|\hat{A}_\alpha^\dagger|\epsilon'\rangle\langle\epsilon'|\hat{A}_\beta|e\rangle\langle e|\otimes\mathbb{I}_N. \quad \text{(B2)}
\end{aligned}$$

Applying *condition II* on the energy difference $\omega-\omega'$ as for Assertion (2), we find that $n^\epsilon = n^e$ and the commutator in Eq. (B2) vanishes, proving Assertion (3). Assertion (4) is verified analogously, and we have proven Proposition 1.

APPENDIX C: JORDAN-WIGNER TRANSFORMATIONS

In this Appendix we briefly present the well-known Jordan-Wigner technique [51,53] to represent spins as fermions, and we show how to employ it to recast the Hamiltonian of an excitation-preserving spin chain in a quadratic fermionic Hamiltonian. Given a system of M spins, we apply the following Jordan-Wigner transformations to write each spin operator as a function of fermionic operators:

$$\begin{aligned}
\sigma_k^z &= c_k^\dagger c_k - \tfrac{1}{2}, \\
\sigma_k^+ &= c_k^\dagger\, e^{i\pi\sum_{l<k} n_l}, \\
\sigma_k^- &= c_k\, e^{-i\pi\sum_{l<k} n_l}.
\end{aligned} \tag{C1}$$

The reader can verify the anticommutation rules $\{c_j, c_k^\dagger\} = \delta_{jk}, \{c_j, c_k\} = 0$.

Let us now suppose that the spins are interacting in an excitation-preserving chain, with Hamiltonian

$$H_{SC} = \sum_{k=1}^M \frac{\omega_k}{2}\sigma_k^z + \sum_{k=1}^{M-1} J_k(\sigma_{k+1}^+\sigma_k^- + \text{H.c.}). \tag{C2}$$

Using the Jordan-Wigner transformations in Eq. (C1), we can express it as

$$\begin{aligned}
H_{SC} &= \sum_{k=1}^M \frac{\omega_k}{2}\left(c_k^\dagger c_k - \frac{1}{2}\right) \\
&\quad+ \sum_{k=1}^{M-1} J_k(c_{k+1}^\dagger e^{i\pi n_k} c_k^- + \text{H.c.}),
\end{aligned} \tag{C3}$$

where we have used $[e^{i\pi\sum_{l<k} n_l}, c_k] = 0$ for $k \geqslant l$. Noticing that $e^{i\pi n_k} c_k|0\rangle_k = 0$ and $e^{i\pi n_k} c_k|1\rangle_k = c_k|1\rangle_k$, we observe that the phase $e^{i\pi n_k}$ has no effects and can be removed from the Hamiltonian. Therefore, Eq. (C3) is quadratic in the fermionic operators and can be recast in the form of Eq. (16), thus being suitable for the analysis in Sec. III.

APPENDIX D: TWO COUPLED SPINS AS FREE FERMIONS

In this Appendix we show how to employ the Jordan-Wigner transformations to write a system of two coupled spins as noninteracting fermions (part of the discussion was already addressed in Ref. [70]). For convenience, we rewrite the Jordan-Wigner transformations Eq. (C1) for two spins as

$$\begin{aligned}
\sigma_1^z &= 1 - 2c_1^\dagger c_1, \qquad & \sigma_2^z &= 1 - 2c_2^\dagger c_2, \\
\sigma_1^x &= c_1^\dagger + c_1, \qquad & \sigma_2^x &= (1 - 2c_1^\dagger c_1)(c_2^\dagger + c_2),
\end{aligned} \tag{D1}$$

where c_1 and c_2 are fermionic operators. The free Hamiltonian of the coupled qubits, given in Eq. (21), is now transformed following Eq. (D1):

$$\begin{aligned}
H_S &= \frac{\omega_1}{2}(1 - 2c_1^\dagger c_1) + \frac{\omega_2}{2}(1 - 2c_2^\dagger c_2) \\
&\quad+ \lambda(c_1^\dagger - c_1)(c_2^\dagger + c_2).
\end{aligned} \tag{D2}$$

In order to diagonalize H_S written in terms of fermionic operators, we first perform the Bogoliubov transformation

$$\begin{aligned}
c_1 &= \cos\theta\,\xi_1 + \sin\theta\,\xi_2^\dagger, \\
c_2 &= \cos\theta\,\xi_2 - \sin\theta\,\xi_1^\dagger,
\end{aligned} \tag{D3}$$

and then the rotation

$$\begin{aligned}
\xi_1 &= \cos\phi\, f_1^\dagger + \sin\phi\, f_2^\dagger, \\
\xi_2 &= \cos\phi\, f_2^\dagger - \sin\phi\, f_1^\dagger.
\end{aligned} \tag{D4}$$

Let us now write Eq. (D2) after having applied the Bogoliubov transformation:

$$\begin{aligned} H_S = &+\frac{\omega_1}{2}[1-2(\cos^2\theta\,\xi_1^\dagger\xi_1+\sin^2\theta\,\xi_2\xi_2^\dagger+\sin\theta\cos\theta(\xi_2\xi_1+\text{H.c.}))] \\ &+\frac{\omega_2}{2}[1-2(\cos^2\theta\,\xi_2^\dagger\xi_2+\sin^2\theta\,\xi_1\xi_1^\dagger+\sin\theta\cos\theta(\xi_2\xi_1+\text{H.c.}))] \\ &+\lambda[2\cos\theta\sin\theta(\xi_1\xi_1^\dagger+\xi_2\xi_2^\dagger)-2\cos\theta\sin\theta+(\cos^2\theta-\sin^2\theta)(\xi_2\xi_1+\text{H.c.})+(\xi_1^\dagger\xi_2+\text{H.c.})]. \end{aligned} \tag{D5}$$

We set θ so as to delete all the double-excitation terms in Eq. (D5):

$$-\omega_+\sin\theta\cos\theta+\lambda(\cos^2\theta-\sin^2\theta)=0\Rightarrow\tan 2\theta=\frac{2\lambda}{\omega_+}, \tag{D6}$$

with $\omega_+=\omega_1+\omega_2$.

Using the condition in Eq. (D6), we now write H_S after having performed the rotation:

$$\begin{aligned} H_S = &+\frac{\omega_1}{2}[1-2((\sin^2\theta\sin^2\phi-\cos^2\theta\cos^2\phi)f_1^\dagger f_1 \\ &+(\sin^2\theta\cos^2\phi-\cos^2\theta\sin^2\phi)f_2^\dagger f_2 \\ &+\sin\phi\cos\phi(f_1f_2^\dagger+\text{H.c.})+\cos^2\theta)] \\ &+\frac{\omega_2}{2}[1-2((\sin^2\theta\sin^2\phi-\cos^2\theta\cos^2\phi)f_2^\dagger f_2 \\ &+(\sin^2\theta\cos^2\phi-\cos^2\theta\sin^2\phi)f_1^\dagger f_1 \\ &-\sin\phi\cos\phi(f_1f_2^\dagger+\text{H.c.})+\cos^2\theta)] \\ &+\lambda[\sin 2\theta(f_1^\dagger f_1+f_2^\dagger f_2)+\sin 2\phi(f_1^\dagger f_1-f_2^\dagger f_2) \\ &+(\cos^2\phi-\sin^2\phi)(f_1f_2^\dagger+\text{H.c.})-\sin 2\theta]. \end{aligned} \tag{D7}$$

In order to eliminate the remaining cross terms, we set the value of ϕ:

$$-\omega_-\sin\phi\cos\phi+\lambda(\cos^2\phi-\sin^2\phi)=0\Rightarrow\tan 2\phi=\frac{2\lambda}{\omega_-}, \tag{D8}$$

with $\omega_-=\omega_1-\omega_2$.

By employing the relations $\cos^2\alpha\cos^2\beta-\sin^2\alpha\sin^2\beta=(\cos 2\alpha+\cos 2\beta)/2$ and $\cos^2\alpha\sin^2\beta-\sin^2\alpha\cos^2\beta=(\cos 2\alpha-\cos 2\beta)/2$, we finally obtain the Hamiltonian

$$H_S=E_1(2f_1^\dagger f_1-1)+E_2(2f_2^\dagger f_2-1), \tag{D9}$$

where

$$E_1=\frac{\sqrt{\lambda^2+\omega_+^2/4}+\sqrt{\lambda^2+\omega_-^2/4}}{2},\quad E_2=\frac{\sqrt{\lambda^2+\omega_+^2/4}-\sqrt{\lambda^2+\omega_-^2/4}}{2}. \tag{D10}$$

We can now proceed to write the spin operators in terms of the fermionic operators. Let us start with σ_1^x:

$$\sigma_1^x=\cos(\theta+\phi)(f_1^\dagger+f_1)+\sin(\theta+\phi)(f_2^\dagger+f_2). \tag{D11}$$

By noticing that $(1-2c_1^\dagger c_1)(1-2c_2^\dagger c_2)(c_2-c_2^\dagger)=\sigma_2^x$, we can readily obtain

$$\sigma_2^x=\cos(\theta-\phi)P(f_2^\dagger-f_2)+\sin(\theta-\phi)P(f_1^\dagger-f_1), \tag{D12}$$

where

$$P=(1-2c_1^\dagger c_1)(1-2c_2^\dagger c_2)=(2f_1^\dagger f_1-1)(2f_2^\dagger f_2-1) \tag{D13}$$

is the parity operator, which tells us whether the number of excitations in the system is even or odd. The Hamiltonian H_S conserves the parity of the excitation number, i.e., $[H_S,P]=0$, thus we are sure that P has the form presented in Eq. (D13).

The form of the operators σ_1^z and σ_2^z is more involved, since they inevitably contain the “double emission” and “double absorption” terms f_1f_2 and $f_1^\dagger f_2^\dagger$, which we could find in the coupling of the original Hamiltonian Eq. (21) $\lambda\sigma_1^x\sigma_2^x$. In some particular scenarios, it is possible to perform a rotating wave approximation on such direct interaction, and to write it as $\lambda(\sigma_1^+\sigma_2^-+\sigma_1^-\sigma_2^+)$, which does not add excitations into the system. In this case, diagonalizing the system Hamiltonian is easier and can be done by just a single rotation [4]. Anyway, with the aim at a more complete description, we keep the counter-rotating terms in the Hamiltonian and we write the operators as

$$\begin{aligned} \sigma_1^z = &(\cos 2\theta+\cos 2\phi)f_1^\dagger f_1+(\cos 2\theta-\cos 2\phi)f_2^\dagger f_2 \\ &-\cos 2\theta-2[\cos\phi\sin\phi(f_1f_2^\dagger+\text{H.c.}) \\ &+\cos\theta\sin\theta(f_1f_2+\text{H.c.})]. \\ \sigma_2^z = &(\cos 2\theta+\cos 2\phi)f_2^\dagger f_2+(\cos 2\theta-\cos 2\phi)f_1^\dagger f_1 \\ &-\cos 2\theta-2[\cos\phi\sin\phi(f_1^\dagger f_2+\text{H.c.}) \\ &+\cos\theta\sin\theta(f_1f_2+\text{H.c.})]. \end{aligned} \tag{D14}$$

Finally, we find the new basis that diagonalizes H_S as a function of the canonical basis $\{|11\rangle,|10\rangle,|01\rangle,|00\rangle\}$, which corresponds respectively to both spins up, first spin up and second down, etc. To represent the excitation basis of each couple of fermionic operators, we employ a subscript indicating to which operator we are referring, while we do not use subscripts for the canonical basis; for instance from Eq. (D1) we understand that

$$\begin{aligned} |00\rangle_c=|11\rangle,\quad |01\rangle_c=|10\rangle, \\ |10\rangle_c=|01\rangle,\quad |11\rangle_c=|00\rangle. \end{aligned} \tag{D15}$$

From Eq. (D4) we see that the vacuum state of f_1, f_2 is the fully excited state of ξ_1,ξ_2, i.e., $|00\rangle_f=|11\rangle_\xi$. In order to find $|00\rangle_f$, i.e., the ground state of H_S, we thus impose that $\xi_1^\dagger$ and $\xi_2^\dagger$ applied on a linear combination of the states in Eq. (D15) read 0. For instance,

$$\xi_1^\dagger \sum_{\alpha,\beta=0,1} a_{\alpha\beta}|\alpha\beta\rangle_c = 0$$
$$\Rightarrow \cos\theta\, a_{00} = -\sin\theta\, a_{11}, \quad a_{01} = 0. \tag{D16}$$

Finally we have

$$|00\rangle_f = +\sin\theta|11\rangle - \cos\theta|00\rangle. \tag{D17}$$

The remaining states are obtained by applying $f_1^\dagger$ and $f_2^\dagger$ on the ground state, and they read:

$$|01\rangle_f = -\sin\phi|10\rangle + \cos\phi|01\rangle,$$
$$|10\rangle_f = -\cos\phi|10\rangle - \sin\phi|01\rangle, \tag{D18}$$
$$|11\rangle_f = +\cos\theta|11\rangle + \sin\theta|00\rangle.$$

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