Steady-State Coherences by Composite System-Bath Interactions

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(Received 28 February 2018; revised manuscript received 1 June 2018; published 15 August 2018)

We identify sufficient conditions on the structure of the interaction Hamiltonian between a two-level quantum system and a thermal bath that, without any external drive or coherent measurement, guarantee the generation of steady-state coherences (SSC). The SSC obtained this way, remarkably, turn out to be independent of the initial state of the system, which could therefore be taken as initially incoherent. We characterize in detail this phenomenon, first analytically in the weak coupling regime for two paradigmatic models, and then numerically in more complex systems without any assumption on the coupling strength. In all of these cases, we find that SSC become increasingly significant as the bath is cooled down. These results can be directly verified in many experimental platforms.

DOI: 10.1103/PhysRevLett.121.070401

Standard textbook quantum mechanics deals with closed systems and their coherent unitary evolution. However, every realistic quantum system has to be considered as open in light of its unavoidable interaction with its surroundings. The resulting reduced nonunitary system takes into account irreversible processes, such as decoherence and dissipation [1,2]. The former, especially, still remains among the major obstacles to all of the countless applications relying on the maintenance and exploitation of quantum coherences, ranging from quantum metrology [3] and state engineering [4], to even relatively far fields such as quantum thermodynamics [5] and quantum biology [6,7]. Because of this prominence, a lot of effort thus has been devoted to conceive strategies to oppose or even neutralize the detrimental effects of environmental couplings, e.g., error-correction schemes [8], dynamical decoupling [9], and quantum feedback control [10], just to mention a few.

Currently, the theory of coherence represents a wide research field, encompassing theoretical developments of a resource theory of coherences [11], characterization of suitable quantifiers and measures of coherence [12], investigation of coherence dynamics [13] and experimental applications [14]. Recently, it was also shown that, under specific conditions on the parameters determining the dynamics, a spin undergoing a pure-dephasing evolution may, in the long-time dynamics, retain some of its initial coherences in the energy eigenbasis [15–17]. In particular, Addis *et al.* provided a clear-cut connection between this phenomenon, which they named coherence trapping, and the properties of the environmental spectrum [16]: while its temperature and low-frequency part determines the partial survival or complete erasure of the initial coherences, its high-frequency band dictates their maximum attainable amount.

The main limitations of such a result are twofold. The first one is that it relies on the specific model and interaction considered, i.e., a pure-dephasing spin boson [2]. When more general dissipative spin-boson dynamics are taken into account [18], i.e., when the interaction does not commute anymore with the system's bare Hamiltonian, all of the coherences inevitably vanish in the long-time limit, irrespective of the type of environment considered. Individual attempts at generalizing this result and extending it to other models have been pursued in [19], where qubit states initially correlated with the environment were considered, and in [20], where a slow down of the coherences decay was characterized for two qubits interacting with a harmonic oscillator. In both cases, however, additional resources to achieve steady-state coherences (SSC), such as initial correlations or a mediating system, were employed. The second fundamental limitation is its initial-state dependence: coherence trapping dictates a way to preserve, by means of clever engineering of the environment, a fraction of initial coherences which, if not present, are not thus generated by this process. This process thus requires state preparation of a coherent superposition.

In this Letter, we aim to remove these two significant constraints and instead provide sufficient conditions concerning the structure of the system-bath interaction Hamiltonian that guarantees the formation (and not mere trapping) of SSC in a generic two-level system, independent of its initial state. In this case, no additional systems, state preparations, or measurement procedures are required. It is well known that quantum coherence can be induced by means of external classical driving [21] or by coherent measurement [22,23]. The only resource we employ here are composite unitary system-bath dynamics, achievable in many experimental platforms. In particular, we will give conclusive evidence of the following statement (see also the schematics in Fig. 1).

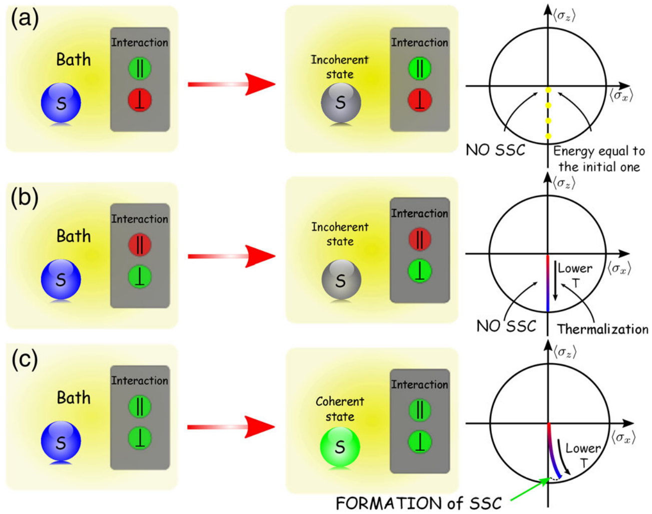

FIG. 1. A two-level system is put in contact with a thermal bath until the steady state is reached. The steady-state solution is shown in the right column using a xz planar section of the Bloch sphere, where, for illustrative purposes, we have assumed the coherences to be real. In the case of a interaction parallel to $\mathcal{H}_S$, (a) the steady-state solution is an incoherent state depicted on the z axis (yellow points), relative to a final energy which is equal to the initial one. In the case of an interaction orthogonal to $\mathcal{H}_S$, (b) the system will thermalize with the bath and SSC will not be present, its steady state thus again being given by a point on the z axis determined by the Boltzmann factor relative to the temperature T. However, when the interaction is a linear combination of parallel and orthogonal interactions, (c) the steady state solution acquires a deviation from the thermal state, due to the formation of coherences, which is in general increasingly pronounced as long as the bath is cooled down.

Observation: Consider a two-level system interacting with a single thermal environment, such that the total Hamiltonian is $\mathcal{H} = \mathcal{H}_S + \mathcal{H}_E + \mathcal{H}_{\rm SE}$. The interaction Hamiltonian $\mathcal{H}_{\rm SE}$ is considered to be a Hermitian operator of the form $\mathcal{H}_{\rm SE} = \sum_j O_{S,j} \otimes b_E + \text{H.c.}$, with $O_{S,j}$ denoting system's operators and $b_E = \sum_k g_k b_k$ denoting the multimode environmental annihilation operator.

Let $\mathcal{H}_{\rm SE}^{\parallel \mathcal{H}_S} \equiv h_S^{-1} \mathrm{Tr}_S[\mathcal{H}_S \sum_j O_{S,j}] \mathcal{H}_S \otimes b_E + \text{H.c.}$ (with $h_S \equiv \mathrm{Tr}_S[\mathcal{H}_S^2]$) denote the projection of the interaction Hamiltonian parallel to $\mathcal{H}_S$ (according to the Hilbert-Schmidt scalar product [2]), and let $\mathcal{H}_{\rm SE}^{\perp \mathcal{H}_S} \equiv \mathcal{H}_{\rm SE} - \mathcal{H}_{\rm SE}^{\parallel \mathcal{H}_S}$ denote its orthogonal complement.

If the interaction Hamiltonian has both nonzero projections over the parallel and orthogonal components with respect to $\mathcal{H}_S$, i.e., if $\mathcal{H}_{\rm SE} = \mathcal{H}_{\rm SE}^{\parallel \mathcal{H}_S} + \mathcal{H}_{\rm SE}^{\perp \mathcal{H}_S}$, then the two-level system will show SSC with respect to the eigenbasis of $\mathcal{H}_S$, independent of the initial state.

Moreover, we will show that the SSC generated this way can be generically enhanced simply when the bath is cooled down, and that they decay slowly with increasing temperature, thus ensuring their possible observation even for a nonzero temperature in experimental setups. These results apply to a wide class of systems and interaction Hamiltonians, and here, we will explicitly provide a paradigmatic analysis for experimentally relevant examples of them. The implications of this result pave the way for optimization of the system-bath interaction in experimental platforms in order to achieve autonomous SSC.

Let us start by considering a two-level system coupled to a thermal bosonic bath such that the total Hamiltonian is given by

$$\mathcal{H} = \frac{\omega_0}{2}\sigma_z + \sum_k \omega_k b_k^\dagger b_k + (f_1\sigma_z + f_2\sigma_x) \otimes B_E, \quad (1)$$

with $\sigma_{x,y,z}$ being the usual Pauli matrices, $B_E = \sum_k g_k (b_k + b_k^\dagger)$ representing the multimode quadrature operator, with $\{b_k^\dagger, b_k\}_k$ denoting the family of bosonic creation and annihilation operators, and $f_{1,2}$ being two generic coupling constants independent on the bath modes k. We stress again that the crucial point is that the system-bath interaction Hamiltonian satisfies the condition stated in the Proposition. The parallel projection $\mathcal{H}_{\rm SE}^{\parallel \mathcal{H}_S} = f_1 \sigma_z \otimes B_E$ induces pure dephasing dynamics on the reduced system, while the orthogonal projection $\mathcal{H}_{\rm SE}^{\perp \mathcal{H}_S} = f_2 \sigma_x \otimes B_E$ will generate dynamics involving both populations and coherences of the two-level system [2,18]. In the following calculations, we will assume the system and the environment to be weakly coupled and starting in a product state $\rho_{\rm SE}(0) = \rho_S(0) \otimes \rho_\beta$, with $\rho_\beta \equiv Z^{-1} e^{-\beta \mathcal{H}_E}$ being the Gibbs state at inverse temperature $\beta = (k_B T)^{-1}$ ($Z = \mathrm{Tr}_E[e^{-\beta \mathcal{H}_E}]$, $\mathcal{H}_E = \sum_k \omega_k b_k^\dagger b_k$). When $f_2 \to 0$, we retrieve pure dephasing dynamics [2], while for $f_1 \to 0$, the evolution retraces the usual decoherent dynamics of a dissipative spin-boson [2,18,24]. By means of standard techniques (i.e., time-convolutionless expansion of the dynamical generator up to second order in the coupling constant [2]), we derived a time-dependent non-Markovian master equation for the system's density operator, and then, from the latter, we obtained the equations of motion for the three components of the Bloch vector $\mathbf{v}(t)$, defined through the relation $\rho_S(t) = \frac{1}{2}(\mathbb{1}_2 + \mathbf{v}(t) \cdot \boldsymbol{\sigma})$, with $v_{x,y,z}(t) = \mathrm{Tr}_S[\sigma_{x,y,z}\rho_S(t)]$. In particular, $v_3(t)$ gives the population imbalance of the qubit while $v_{1,2}(t)$ denote the real and imaginary parts of coherences in the σ_z basis, respectively. The interested reader is referred to the Supplemental Material [25] (SM, Section A) for a detailed derivation and additional comments concerning the dynamics of such a system.

Since for many practical purposes it is easiest to exploit the steady-state properties of a system, we have focused on the long-time limit. The resulting steady-state solutions for $v_{1,2}$ characterize SSC, and they turn out to be given by [see the SM, Eq. (42)]

$$\bar{v}_1 = \frac{f_1 f_2 [\Delta_1 \tanh(\frac{\omega_0}{2T}) + 4\lambda\Omega\Gamma(s) + \Delta_2]}{\omega_0 + f_2^2 \Delta_1}, \quad \bar{v}_2 = 0, \quad (2)$$

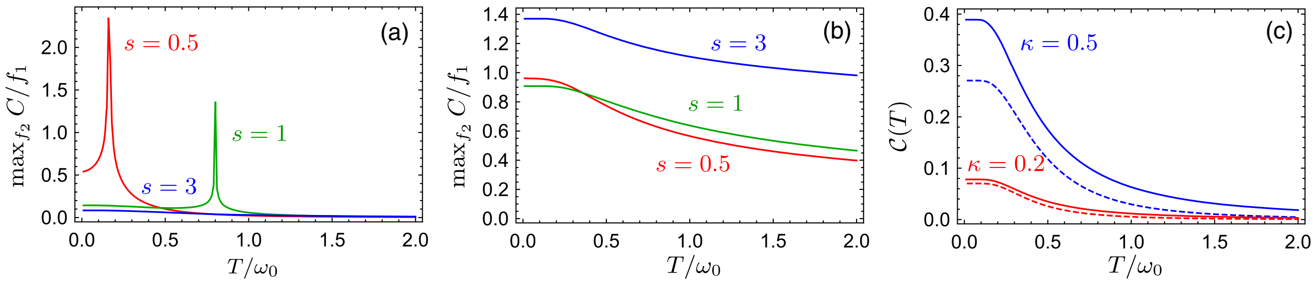

FIG. 2. Temperature dependence of SSC: (a) Eq. (4) for $\lambda = 10^{-2}\omega_0$, and cut-off frequency $\Omega = 5\omega_0$; (b) Eq. (78) of the SM for the same choice of parameters; (c) the coherence measure $\mathcal{C}$ for different couplings κ between the qubit and its effective bath, namely a harmonic mode, in turn coupled to a thermal bath (solid lines), and a spin chain in turn coupled to a thermal bath (dashed lines), see Section E of the SM.

where $\Gamma(x)$ is the Euler's function and where we have defined (omitting for brevity their parameter dependence)

$$\Delta_1(T,\Omega) = -2\int_0^{+\infty} d\omega J_{\mathrm{eff}}(\Omega,T)\left(\mathcal{P}\frac{1}{\omega+\omega_0} - \mathcal{P}\frac{1}{\omega-\omega_0}\right),$$
$$\Delta_2(\Omega) = -2\int_0^{+\infty} d\omega J(\omega)\left(\mathcal{P}\frac{1}{\omega+\omega_0} + \mathcal{P}\frac{1}{\omega-\omega_0}\right), \quad (3)$$

with $\mathcal{P}$ standing for Cauchy principal value, $J(\omega)$ denoting the spectral density of the bath, and $J_{\mathrm{eff}}(\omega,T) \equiv J(\omega)\coth[(\omega_0/2T)]$ being the so-called effective spectral density [24]. The former has been taken to be of the general Ohmic-dependent form $J(\omega) = \lambda(\omega^s/\Omega^{s-1})e^{-\omega/\Omega}$, with λ being a coupling constant, Ω the cut-off frequency, and s the Ohmicity parameter ruling over the low-frequency behavior. The latter is known to lead to a sub-Ohmic spectrum for $s < 1$, to an Ohmic one for $s = 1$, and finally, to a super-Ohmic spectrum for $s > 1$ [18]. As can be immediately seen from Eq. (2), if either one of the two couplings $f_{1,2}$ goes to zero, $\bar{v}_1$ vanishes. It is then the simultaneous presence of both terms in the interaction Hamiltonian (1) that guarantees the occurrence of SSC. Moreover, it is worth pointing out that the reason why only $\bar{v}_1$ has survived in the steady state while $\bar{v}_2 = 0$ is only due to the specific choice of the structure of Eq. (1), whose orthogonal projection $\mathcal{H}_{\mathrm{SE}}^{\perp\mathcal{H}_s}$ was proportional to σ_x. An exchange $\sigma_x \to \sigma_y$ in such an interaction Hamiltonian produces a corresponding nonzero value of $\bar{v}_2$ and $\bar{v}_1 = 0$.

Finally, it is central to notice that the result in (2) is remarkably independent of the initial state of the system. This draws a neat line of distinction with the previous phenomenon of coherence trapping studied, e.g., in [16]. While in their case, an opportunely engineered environment and interaction was exploited in order to make a fraction of the initial coherences to survive the dephasing process (due to the damping coefficient going to zero in a finite time interval), in our case nonzero SSC have been built up even in the case that the system starts in an incoherent state. We emphasize that the generation of such SSC stems purely from the system-bath interaction, and it is thus autonomous, in the sense that no coherent driving or measurement is introduced in the scheme.

To further discuss the above result, and in light of comparisons in the subsequent models, we will employ the l_1- norm of coherence $\mathcal{C} = \sqrt{\bar{v}_1^2 + \bar{v}_2^2}$, first introduced in [27], which can be shown to satisfy all of the properties to be considered as a valid coherence measure [28]. First of all, one can immediately notice that $\bar{v}_1$ is linear in f_1, i.e., the strength determining the dephasing, and so $\mathcal{C}$ will be given in units of it. It is important to keep in mind, however, that the range of f_1 remains firmly limited by the weak-coupling condition according to which $\lambda f_{1,2} \ll \omega_0$ [2]. The maximum of $\mathcal{C}$ with respect to f_2 can be instead analytically calculated, and thus one obtains

$$\max_{f_2} \mathcal{C}/f_1 = \left|\frac{[\Delta_1 \tanh(\frac{\omega_0}{2T}) + 4\lambda\Omega\Gamma(s) + \Delta_2]}{2\sqrt{\omega_0\Delta_1}}\right|. \quad (4)$$

Two important general features of Eq. (4), with respect to Ω and T, can be seen to be generally valid, irrespective of the Ohmicity parameter s. First of all, for any fixed value of the temperature, the coherence measure turns out to be a nondecreasing function of the cutoff frequency Ω. This is because, in this model, a larger Ω reflects a higher value of $J(\omega_0)$. More interestingly, it turns out that the SSC are progressively enhanced as the bath is cooled down, reaching its maximum (as a function of T for any fixed Ω) for $T \to 0$. On the other side, they are found to vanish in the high-temperature limit, consistent with the intuition that a more "classical" hot bath prevents the observation of such phenomenon. However, remarkably in view of experimental applications, the decay of generated SSC with increasing T is slow, thus allowing for their observation even at nonzero bath temperatures. Alongside these general properties, the remaining parameter s ruling over the low-frequency shape of the spectrum induces a different behavior of Eq. (4), whether $s \le 1$ or $s > 1$. For further details, see Sec. A.4 of the SM.

The Ohmic and sub-Ohmic cases.—Performing a first-order Taylor expansion of the integrands of (3) around

$\omega = \omega_0$, allows us to realize that there is a pole of the first order in these along the so-called resonance curve [24], implicitly defined by the condition $\partial_\omega J_{\text{eff}}(\omega, T)|_{\omega=\omega_0} = 0$. The resonance curve physically indicates a match between the system's frequency ω_0 and the frequency $\omega_{\max}$ for which the spectrum reaches its maximum, i.e., such that $\partial_\omega J_{\text{eff}} = 0$. When such a dominant environmental frequency $\omega_{\max}$ coincides with ω_0, i.e., is resonant with the system, then the system practically interacts with a locally flat spectrum, the latter notoriously leading to a Markovian dynamics [24]. The enhancement of SSC along the resonance curve can be seen in Fig. 2(a), where the "spike" of (4), plotted as function of the bath temperature T for a fixed $\Omega = 5\omega_0$, is located on a point of that curve. The resonance curve thus allows a relatively higher coherence for the same f_1 and optimized f_2. The sub-Ohmic case does not qualitatively differ from the Ohmic case, as the resonance condition highlighted above still plays the same role here; see the red curve in Fig. 2(a). A more thorough discussion can be found in Section A.4 of the SM.

Super Ohmic case.—The singular behavior of the integrand of $\Delta_{1,2}$ in Eq. (3) disappears when $s \geq 2$. The coherence measure consequently shows a more regular behavior, as shown by the absence of resonance peaks of the blue line in Fig. 2(a), which refers to the case $s = 3$. It is worth mentioning that such a spectral density is of prominent importance in the context of polarons, when defects or electron tunneling in a solid coupled to a three-dimensional phononic bath is considered [18].

Since many physical systems, especially in quantum optics, are described by interaction Hamiltonians in the so-called rotating wave approximation (RWA), we now reconsider the same two-level system and bosonic bath as above, but this time coupled according to

$$\mathcal{H}_{\text{SE}} = f_1 \sigma_z \otimes B_E + f_2(\sigma_+ \otimes b_E + \sigma_- \otimes b_E^\dagger), \quad (5)$$

with $B_E = b_E + b_E^\dagger$ and $b_E = \sum_k g_k b_k$. We emphasize that the interaction in Eq. (5), despite being in a RWA, still satisfies the Observation. Performing the same master-equation based analysis, in this case we also obtain nonzero SSC, which remarkably shows the same qualitative features and behavior as in the previous model (see Sec. B of the SM for quantitative results and discussions). The behavior of the maximum coherence measure as a function of the bath temperature T is shown in Fig. 2(b), for the same values of Ω and s used for the previous model in Fig. 2(a). A comparison between the two plots immediately shows that the general trend of SSC to increase when T decreases is also found in this model. At variance with the previous case, however, all of the singular behavior of the steady state complements $\bar{v}_{1,2}$ at the resonance frequency ω_0 and is removed for every value of s, as detailed and discussed in Sec. B.4 of the SM. This reflects in the absence of enhancement peaks of SSC, even for Ohmic or sub-Ohmic spectral densities.

To provide a complete picture, we have further investigated what happens if we split the two projections $\mathcal{H}_{\text{SE}}^{\parallel \mathcal{H}_S, \perp \mathcal{H}_S}$ of an interaction Hamiltonian of the form Eq. (1) and attribute them to two separate independent thermal baths attached to the system (their temperature being arbitrary and eventually different), neither of which will therefore satisfy the Observation. It turns out that in this case, all SSC vanish (see Sec. C of the SM), this clearly indicating that the SSC obtained above cannot be equivalently generated through alternate sequences of interactions with independent baths, each one not generating SSC. On the other hand, remarkably, we have checked that the generation of SSC by means of an interaction Hamiltonian of the suitable structure evidenced, e.g., Eqs. (1) and (5), are robust even in the presence of an additional dephasing channel on top of it (see Sec. D of the SM). This represents an important support to the feasibility of an eventual experimental test of such theoretically predicted phenomenon, as in many physical situations there often is an unwanted secondary environment.

Equilibration picture.—An alternative approach, with respect to the master-equation-based one, can also be pursued through the equilibration theory. The latter is based on the strong suggestion, widely assumed in the community of closed quantum many-body systems, that quantum systems coupled to a large thermal bath should equilibrate with it, so that the stationary state is given by the local reduced state of the global Gibbs state, i.e., $\rho_S = \text{Tr}_E[Z^{-1} e^{-\beta \mathcal{H}}]$, with $Z = \text{Tr}_{\text{SE}}[e^{-\beta \mathcal{H}}]$ [29,30]. The global Gibbs state differs from the local Gibbs state due to the presence of the interaction Hamiltonian. While being particularly enhanced in the strong coupling regime, even in the weak-coupling regime the corrections to the thermal state $e^{-\beta \mathcal{H}_S}/\text{Tr}_S[e^{-\beta \mathcal{H}_S}]$ can become significant [31,32]. This approach allows us to characterize only steady-state properties, and moreover, it can work only when the system is coupled to a single thermal bath inducing equilibration. Nevertheless, it proves extremely useful in order to characterize SSC even in strongly coupled systems as well as more complex many-body systems. First of all, we have then employed a perturbative expansion up to the second order in the coupling strength of the local reduced state of the global Gibbs state, in the same spirit as done in [33], for the model described by Eq. (1) (see the SM, Sec. E). The results obtained through this different approach have notably confirmed all of the above conclusions.

Finally, we employed the equilibration method to access SSC in different models. In particular, we have first considered a qubit, the subsystem of interest, coupled to a harmonic oscillator through an interaction having the crucial composite structure, put in evidence in this work and equilibrated by means of an interaction with a thermal reservoir. Subsequently we also studied the case where the role of the harmonic oscillator is taken by another two-level system; the reader is referred to Sec. E of the SM for all of the details. In both cases, a fully numerical approach has been pursued, and thus no weak coupling assumption has been invoked. In Fig. 2(c), we show the temperature dependence of the coherence measure $\mathcal{C}$ for different values of the coupling strength κ. Solid lines refer to the first model [with the Hamiltonian given by Eq. (107) of the SM], while dashed lines refer to the second one [with the Hamiltonian given by Eq. (108) of the SM]. A comparison between the curves in Figs. 2(a), 2(b), and 2(c) shows a great consistency in the behavior of SSC with respect to T, namely its enhancing for a cold bath, thus supporting the feasibility of the formation of SSC for different experimental situations. Finally, this trend of SSC is, remarkably, left significantly unchanged even outside the weak coupling regime, as highlighted in Fig. 2(c) by the choice $\kappa = 0.5\omega_0$.

In conclusion, we have provided sufficient descriptions concerning the structure of the interaction Hamiltonian that allows the formation of steady-state coherences in a generic two-level quantum system coupled to a generalized thermal bath. The SSC obtained this way are remarkably independent of the initial state of the system, so that this scheme can be used to obtain coherences even from an initially purely incoherent system state, and they are generally enhanced as the bath temperature is lowered. Interesting outlooks range from theoretical to experimental. On the experimental side, the results presented in this Letter spur the immediate possibility of generating and observing autonomous SSC, for the first time, in many platforms, such as trapped ions [34,35] or superconducting circuits [36–40]. On the other hand, it will be interesting to investigate the generalization to higher dimensional systems and the situation where two thermal baths at different temperatures are attached to the system through interaction Hamiltonians all of the composite form as, e.g., in Eq. (1) or Eq. (5), thus leading to a nonequilibrium steady-state solution (NESS).

The Authors acknowledge the support of the Czech Science Foundation (GACR) (Grant No. GB14-36681G). R. F. acknowledges funding from the MEYS and from the European Union's Horizon 2020 research and innovation framework programme under Grant agreement No. 731473.

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