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Non-Markovian effects in electronic and spin transport

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We derive a non-Markovian master equation for the evolution of a class of open quantum systems consisting of quadratic fermionic systems coupled to wideband reservoirs. This is done by providing an explicit correspondence between master equations and nonequilibrium Green's function approaches. Our findings permit us to address non-Markovian regimes characterized by negative decoherence rates and to characterize the dynamics with respect to a recently proposed measurement of "non-Markovianity." We study the real-time dynamics and the steady-state solution of two illustrative models: a tight-binding electronic model and *XY* spin chains. The rich set of nonequilibrium steady-state phases encountered extends previous results to the non-Markovian regime.

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Interest in out-of-equilibrium processes has been boosted in recent years by considerable experimental progress made in the manipulation and control of quantum systems under nonequilibrium conditions in ultracold gases [1,2], nanodevices [3,4], and spintronic [5,6] setups. This renewed attention in nonequilibrium processes has raised a number of new questions, such as the existence of intrinsic out-of-equilibrium phases and phase transitions [7–11], the definition of effective notions of temperature [12–16], universality of dynamics after quenches [17–21], and thermalization [22–24].

Out-of-equilibrium open quantum systems in contact with thermal reservoirs are fundamentally different from isolated autonomous systems as dissipation is intrinsic to the evolution and thermodynamic imbalances, such as temperature and chemical potential gradients, may induce a finite flow of particles, energy, or spin, which are otherwise conserved quantities. Among the set of theoretical tools available to tackle nonequilibrium quantum dynamics [25,26], the Kadanoff-Baym-Keldysh nonequilibrium Green's function formalism allows for a systematic derivation of the evolution from the microscopic Hamiltonian of the system and its environment. An alternative approach consists of treating open quantum systems with the help of master equations for the reduced density matrix ρ. The formalism is generic as any process describing the evolution of a system and its environment can be effectively described by a master equation of the form [27]

$$\partial_t \rho = \mathcal{L}_t \rho = -i[H(t),\rho] + \sum_\ell \gamma_\ell(t)\left[L_\ell(t)\rho L_\ell^\dagger(t) - \frac{1}{2}\{L_\ell^\dagger(t)L_\ell(t),\rho\}\right], \quad (1)$$

where the L_ℓ's are a suitable set of jump operators, which, without loss of generality, satisfy $\mathrm{tr}\,[L_\ell(t)] = 0$ and $\mathrm{tr}\,[L_{\ell'}^\dagger(t)L_\ell(t)] = \delta_{\ell\ell'}$, and H is the system's Hamiltonian [28]. The specific form of the L_ℓ's is only known for rather specific examples [29–34]. For a generic case, to use this approach on a practical level, one has to rely on various approximations that substantially restrict its applicability range [35,36]. Trace preservation, explicitly respected by Eq. (1), and positivity are essential in order for $\rho(t)$ to represent a physically allowed density matrix. Generic conditions on $L_{\ell'}(t)$ and $\gamma_\ell(t)$ to ensure that the complete positivity of $\rho(t)$ is maintained throughout the evolution are yet unknown [32]. For the case where all decoherence rates are non-negative [$\gamma_\ell(t) \geqslant 0$], positivity can be proven [37,38]. This condition implies that the superoperator $\mathcal{E}_{t,t'}$, evolving the density matrix from t' to t, $\mathcal{E}_{t,t'}(\rho) = T e^{\int_{t'}^{t} d\tau \mathcal{L}_\tau}\rho$ (where T stands for the time-ordered product), is a completely positive map for all $t > t' > 0$. In this case, $\mathcal{E}_{t,t'}$ is also contractive [39], meaning that the distance between two density matrices cannot increase under the time evolution. For time-independent processes, i.e., $\gamma_\ell(t) = \gamma_\ell \geqslant 0$ and $L_\ell(t) = L_\ell$, Eq. (1) reduces to the celebrated Lindblad form [27,37,38], which can be obtained from the microscopic evolution assuming a small system-bath coupling and a Markovian (memoryless) environment. The Markovian assumption has been extremely fruitful, with the Lindblad formalism being widely used to model quantum optics and mesoscopic systems [40–45] and, more recently, quantum transport [8,46–48]. Master equations of the Lindblad form also allow for efficient stochastic simulation techniques using Monte Carlo methods [27,49]. Nonetheless, the evolution of open quantum systems is generically non-Markovian, with some γ_ℓ's assuming negative values. The Lindblad description therefore fails whenever coherent dynamics between the system and environment is essential.

If some of the decoherence rates become negative, although $\mathcal{E}_{t,0}$ is completely positive, $\mathcal{E}_{t,t'}$ for $t' > 0$ might not be so. Thus, not all initial density matrices are allowed starting points for the evolution from t' to t, implying that the process has necessarily some memory. Non-negative decoherence rates can thus be associated with memoryless environments [28,39,50,51]. "Non-Markovianity," i.e., the presence of an environment with a finite memory time, can be detected and measured using recently proposed measurements and witnesses [39,50–55]. Here, we consider the measurement $f_{\mathrm{nM}}(t) = \frac{1}{2}\sum_\ell [|\gamma_\ell(t)| - \gamma_\ell(t)]$, proposed in Ref. [51], that strictly quantifies the degree of non-Markovianity of the dynamics at time t.

In this Rapid Communication we provide a master equation for the class of quadratic fermionic systems coupled to non-interacting wideband reservoirs. This extends the knowledge of the exact form of the jump operators of non-Markovian processes to a wide and important class of models, used to study spin and electronic transport in normal systems and

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superconductors. After providing the explicit form of the jump operators, we show how our results can be applied to treat non-Markovian dynamics in two examples: a tight-binding model and an open *XY* spin chain.

Open quadratic models with wideband reservoirs. We consider a generic quadratic fermionic system coupled to noninteracting fermionic reservoirs (leads) labeled by $\nu = 1,\ldots,m$. The fermionic operators of the system and of the reservoirs are denoted $c_{a=1,\ldots,n}$ and $f_{\nu_{a=1,2,\ldots}}$, respectively. The total Hamiltonian is given by $H = H_c + \sum_\nu H_\nu + H_{c-f}$, where $H_c = \frac{1}{2}\boldsymbol{C}^\dagger \boldsymbol{H}_c \boldsymbol{C}$ is the Hamiltonian of the system, with $\boldsymbol{H}_c$ a single-particle operator and $\boldsymbol{C} = \{c_1,\ldots,c_n,c_1^\dagger,\ldots,c_n^\dagger\}^T$ the Nambu vector. $H_\nu = \sum_i \varepsilon_{\nu_i}(f_{\nu_i}^\dagger f_{\nu_i} - \frac{1}{2})$ is the Hamiltonian of the νth reservoir. The interaction Hamiltonian is given by $H_{c-f} = \sum_{\nu ji}(c_j^\dagger t_{j,\nu_i}^p + c_j t_{j,\nu_i}^h) f_{\nu_i} + \text{H.c.}$ containing generically normal and superconducting hopping terms.

After the coupling is turned on at $t = 0$, we consider the joint system-reservoir evolution of an initially prepared product state. Being a macroscopic system, each reservoir is initially in a Gibbs state specified by β_ν, the inverse temperature, and μ_ν, the chemical potential. The initial density matrix of the system is taken to be of the form $\rho(0) = e^{-\frac{1}{2}\boldsymbol{C}^\dagger \boldsymbol{\Omega}_0 \boldsymbol{C}}/Z$, with $\boldsymbol{\Omega}_0$ a generic single-particle operator.

The Dyson equation on the Keldysh contour can be derived by standard nonequilibrium Green's function techniques [56]. We make a crucial assumption respecting the environment properties—the so-called wideband limit—which amounts to saying that the density of states of each reservoir and their hybridization functions with the system are essentially constant with respect to the system's energy scales. This yields a frequency-independent retarded self-energy, which in the time domain translates to $\boldsymbol{\Sigma}_c^R(t,t') = -i\delta(t-t')\sum_\nu(\boldsymbol{\Gamma}_\nu + \hat{\boldsymbol{\Gamma}}_\nu)$, with $\boldsymbol{\Gamma}_\nu$ the hybridization matrix of reservoir ν and where the operator $.\hat{}.$ denotes particle-hole conjugation. The explicit form of $\boldsymbol{\Gamma}_\nu$ in terms of the system-reservoir couplings is given in the Supplemental Material [57]. The Keldysh component also reduces to a particularly simple form, $\boldsymbol{\Sigma}_c^K(t,t') = -2i\sum_\nu[\boldsymbol{\Gamma}_\nu F_\nu(t-t') - \hat{\boldsymbol{\Gamma}}_\nu \bar{F}_\nu(t-t')]$, where $F_\nu(t) = \int \frac{d\varepsilon}{2\pi}\tanh[\beta_\nu(\varepsilon-\mu_\nu)]e^{-i\varepsilon t}$ encodes the thermodynamic properties of the reservoirs. A different set of assumptions leading to a similar $\boldsymbol{\Sigma}_c^R$ was used in Ref. [58] to study steady-state transport. Within this approximation, the retarded Green's function is simply given by

$$\boldsymbol{G}_c^R(t,t') = -i\Theta(t-t')e^{-i(t-t')\boldsymbol{K}}, \tag{2}$$

where $\boldsymbol{K} = \boldsymbol{H}_c - i\boldsymbol{\Gamma}$ and $\boldsymbol{\Gamma} = \sum_\nu(\boldsymbol{\Gamma}_\nu + \hat{\boldsymbol{\Gamma}}_\nu)$, resembling the solution of a Hamiltonian problem but with $\boldsymbol{K}$ a non-Hermitian operator. The solution for the Keldysh component also considerably simplifies. For simplicity, here we consider equal-time quantities only, defining for that purpose the single-particle correlation matrix $\boldsymbol{\chi}(t) = \langle \boldsymbol{C}(t)\cdot\boldsymbol{C}^\dagger(t)\rangle$ that encodes all information of the equal-time observables. A closed equation for the evolution of $\boldsymbol{\chi}$ can be obtained by using the relation $\boldsymbol{\chi}(t) = \frac{1}{2}[i\boldsymbol{G}_c^K(t,t)+1]$ and Dyson's equation for the Keldysh Green's function, yielding

$$\partial_t\boldsymbol{\chi}(t) = -i\boldsymbol{K}\boldsymbol{\chi}(t) + i\boldsymbol{\chi}(t)\boldsymbol{K}^\dagger + \sum_\nu \boldsymbol{N}_\nu(t), \tag{3}$$

with $\boldsymbol{N}_\nu(t) = \boldsymbol{\Gamma}_\nu + \hat{\boldsymbol{\Gamma}}_\nu + i\{R[(\boldsymbol{K}+\mu_\nu),\beta_\nu,t]\boldsymbol{\Gamma}_\nu + R[(\boldsymbol{K}-\mu_\nu),\beta_\nu,t]\hat{\boldsymbol{\Gamma}}_\nu - \text{H.c.}\}$. The function $R[z,\beta,t] = -i\int_0^t\int\frac{d\varepsilon}{2\pi}dt'\tanh[\beta\varepsilon]e^{-i(z+\varepsilon)(t-t')}$ can be obtained by a suitable regularization of the integral (see the Supplemental Material). The initial condition $\boldsymbol{\chi}(0) = \frac{1}{2}[\tanh(\boldsymbol{\Omega}_0)+1]$ is determined by the density matrix of the system at $t = 0$.

Master equation. We now turn to the alternative approach in terms of the master equation. Under the evolution given by Eq. (1), for a quadratic Hamiltonian and linear jump operators of the form $L_\ell(t) = \sum_i \langle\ell(t)|i\rangle C_i$, an initial Gaussian density matrix remains of the Gaussian form, $\rho(t) = e^{-\frac{1}{2}\boldsymbol{C}^\dagger\boldsymbol{\Omega}(t)\boldsymbol{C}}/Z(t)$, and the single-particle correlation matrix, given by $\boldsymbol{\chi}$, fully encodes all the equal-time properties of the system. Under the Lindblad dynamics $\boldsymbol{\chi}(t)$ evolves as (see Ref. [59] or the Supplemental Material for the derivation)

$$\partial_t\boldsymbol{\chi}(t) = -i\boldsymbol{Q}(t)\boldsymbol{\chi}(t) + i\boldsymbol{\chi}(t)\boldsymbol{Q}^\dagger(t) + \boldsymbol{N}(t), \tag{4}$$

with $\boldsymbol{N}(t) = \sum_\ell \gamma_\ell(t)|\ell(t)\rangle\langle\ell(t)|$ and $\boldsymbol{Q}(t) = \boldsymbol{H}_c(t) - i\frac{1}{2}[\boldsymbol{N}(t) + \hat{\boldsymbol{N}}(t)]$. Identifying the different elements of Eqs. (3) and (4), we obtain $\boldsymbol{Q}(t) = \boldsymbol{K}$ and $\boldsymbol{N}(t) = \sum_\nu \boldsymbol{N}_\nu(t)$. The decoherence rates $\gamma_\ell(t)$ and the vectors $|\ell(t)\rangle$, characterizing the jump operators, can be thus obtained by diagonalizing $\boldsymbol{N}(t)$, given in the Keldysh derivation in terms of the properties of the reservoirs and of the system's Hamiltonian. This procedure explicitly shows how to obtain the master equation describing a non-Markovian process and is the central result of this Rapid Communication. In the following, we discuss the consequences of our findings for dynamics and provide examples. The more general case where the system Hamiltonian and the system-environment couplings depend on time can be straightforwardly obtained and is given in the Supplemental Material for completeness.

It is tempting to analyze independently the contribution $\boldsymbol{N}_\nu(t)$ of each reservoir, however, as these matrices may in general not commute with each other, the dynamical process has to be analyzed globally. Nevertheless, in the case where all contributions $\boldsymbol{N}_\nu(t)$ are positively defined, their sum $\boldsymbol{N}(t)$ is a positively defined matrix and therefore the process is Markovian. Particularly simple examples yielding positively defined contributions arise for time-independent $\boldsymbol{N}_\nu$ in the case of fully empty or fully filled reservoirs [35,36], i.e., $\mu_\nu \to \pm\infty$, for which $\boldsymbol{N}_\nu = 2\hat{\boldsymbol{\Gamma}}_\nu$ and $\boldsymbol{N}_\nu = 2\boldsymbol{\Gamma}_\nu$, respectively, and for infinite temperature, $\beta_\nu \to 0$, for which $\boldsymbol{N}_\nu = \boldsymbol{\Gamma}_\nu + \hat{\boldsymbol{\Gamma}}_\nu$. An open quantum system coupled to a set of such reservoirs is therefore Markovian. Conversely, any Markovian process can be obtained by coupling the system to a set of such simple reservoirs.

In the asymptotic long time limit, $\boldsymbol{N}(t)$ converges to a time-independent matrix $\boldsymbol{N}_\infty$. As the operator $\boldsymbol{K}$ is non-Hermitian, we denote by $|\beta\rangle$ and $\langle\beta'|$ its right and left eigenvectors with eigenvalue λ_β. Stability arguments imply that $\text{Im}\,\lambda_\beta \leqslant 0$. If all the eigenvalues have a nonvanishing imaginary part, a unique steady state exists and the single-particle density matrix is given by $\boldsymbol{\chi}_\infty = -i\sum_{\beta\gamma}|\beta\rangle(\lambda_\beta - \bar{\lambda}_\gamma)^{-1}\langle\beta'|\boldsymbol{N}_\infty|\gamma'\rangle\langle\gamma|$. When all reservoirs are in thermodynamic equilibrium, i.e., $\beta_\nu = \beta$ and $\mu_\nu = \nu$, $\boldsymbol{\chi}_\infty$ reduces to its Gibbs form $\boldsymbol{\chi}_\infty = \frac{1}{2}\{\tanh[\beta(\boldsymbol{H}_c - \mu\boldsymbol{N}_c)]+1\}$ in the limit of vanishing system-reservoir coupling, corresponding to the familiar equilibrium density matrix.

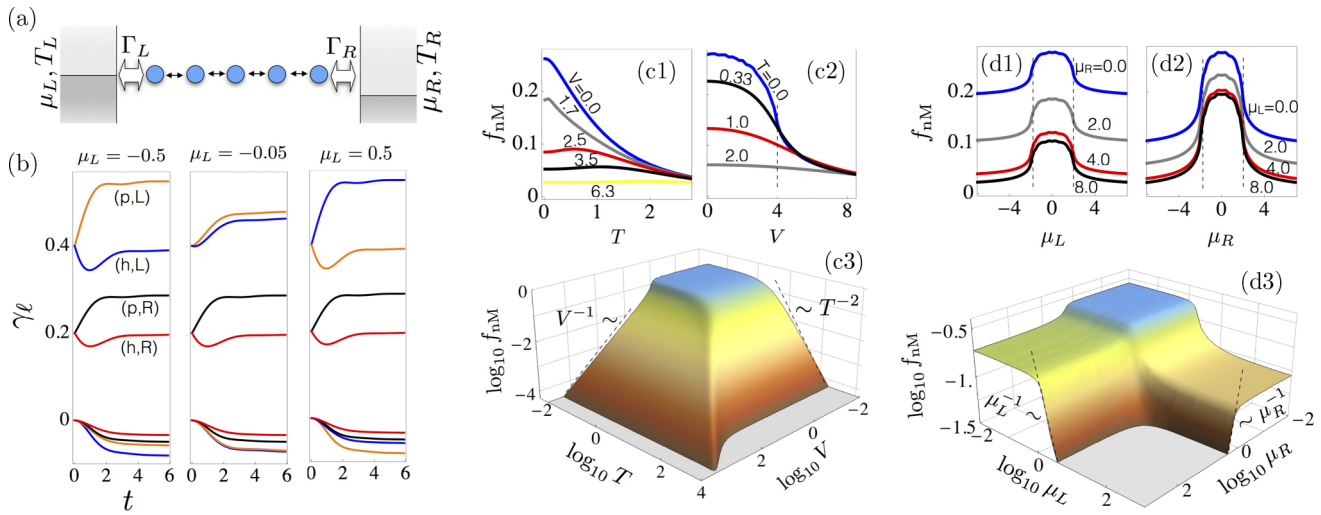

FIG. 1. (Color online) (a) Sketch of the system coupled to thermal reservoirs. (b) Decoherence rates $\gamma_\ell(t)$ as a function of time computed for $M = 50$, $\Gamma_L = 0.4$, $\Gamma_R = 0.2$, $T = 0$, and $\mu_R = 0.5$ for different values of μ_L. The labels $(p/h, L/R)$ refer to the particle or hole nature of the single-particle state $|\ell(t)\rangle$ and to its localization with respect to the boundary. Negative eigenvalues with the same labels as their positive counterparts are depicted in the same line color. (c) Measurement of non-Markovianity $f_{\rm nM}$ for the steady-state process computed for $M = 50$, $\Gamma_L = 0.6$, $\Gamma_R = 0.2$, $T_L = T_R = T$, and $\mu_L = -\mu_R = V/2$ as a function of T and V. (d) The same as in (c) for $T_L = T_R = 0$ as a function of μ_L and μ_R.

Tight-binding chain. In order to demonstrate the previous results, let us consider a tight-binding one-dimensional chain in Fig. 1(a), with $H_c = -\sum_{i=0}^{M-2} c_{i+1}^\dagger c_i + \text{H.c.}$, coupled to two leads at positions 0 and $M-1$ by the hybridization constant Γ_L and Γ_R, respectively.

Figure 1(b) shows the evolution of the decoherence rates $\gamma_\ell(t)$, after the coupling to the reservoirs has been turned on, for different values of μ_L. There are eight nonzero eigenvalues of $\boldsymbol{N}$, arising in positive-negative pairs (see the color code). In the Markovian limit the negative decoherence rates tend to zero. The labels p/h refer to the particle or hole nature of the corresponding eigenvector of $\boldsymbol{N}$, and L/R to their localization near the left or right lead. For $M \to \infty$ we observe that $\boldsymbol{N}_{R/L}|\ell_{L/R}(t)\rangle \to 0$, where $\boldsymbol{N}_\nu(t)|\ell_\nu(t)\rangle = \gamma_{\ell;\nu}(t)|\ell_\nu(t)\rangle$, i.e., for a large size chain the contribution of both reservoirs factorizes and the nonzero eigenvalues of $\boldsymbol{N}$ can be obtained by a direct sum of the spectrum of $\boldsymbol{N}_L$ and $\boldsymbol{N}_R$. This factorization explains that in Fig. 1(b) the R-labeled eigenvalues are unaffected by changes in μ_L. More generally, such a factorization, arising when the special separation between the reservoirs is large, is to be expected for short-range Hamiltonians H_c and allows one to treat the decoherence rates of each reservoir independently. In the present example the structure of $\boldsymbol{N}_\nu$ is particularly simple, corresponding to the two positive and negative eigenvalue pairs in Fig. 1(b). The fact that in Fig. 1(b) the particle or hole nature of the L-labeled eigenvalues is interchanged upon switching $\mu_L \to -\mu_L$ can be seen in the expressions of $|y_\nu^{p/h}\rangle$, together with the fact that $\boldsymbol{K}$ has no anomalous terms.

Figures 1(c) and 1(d) depict the non-Markovianity nature of the steady state as measured by the $f_{\rm nM} = f_{\rm nM}(t \to \infty)$. In Figs. 1(c1)–1(c3) we set $\mu_L = -\mu_R = V/2$, $T_L = T_R = T$, and show $f_{\rm nM}$ as a function of the bias voltage V and temperature T. Figures 1(c1) and 1(c2) show how $f_{\rm nM}$ varies as a function of T and V, respectively. Figure 1(c3) shows a logarithmic plot of $f_{\rm nM}$ for large values of V and T. The Markovian limit, obtained for large values T or V, is attained differently along the two axes, $f_{\rm nM} \propto V^{-1}$ for large V and $f_{\rm nM} \propto T^{-2}$ for large T.

Figure 1(d) shows the variation of $f_{\rm nM}$ with μ_L and μ_R separately at $T_L = T_R = 0$. Figure 1(d3) shows clearly that the Markovian limit is attained only when both chemical potentials are large. This can be understood by the approximate factorization of the eigenvalues of $\boldsymbol{N}$ as a Markovian evolution can only arise when both reservoirs behave as memoryless environments. For $|\mu_{L/R}| \gg |\mu_{R/L}|$, one has $f_{\rm nM} \propto |\mu_{L/R}|^{-1}$.

XY spin chain. In the Markovian limit a number of works have addressed spin and heat transport in spin chains [8,42,46,47,60,61]. Here, we consider an XY spin chain in a transverse field with non-Markovian reservoirs, depicted in Fig. 2(a). The Hamiltonian is given by $H = -\sum_m \frac{J}{2}[(1+\gamma)\sigma_m^x\sigma_{m+1}^x + (1-\gamma)\sigma_m^y\sigma_{m+1}^y] - h\sum_m \sigma_m^z$, where $J = J_c$, $\gamma = \gamma_c$, and $h = h_c$ within the central region. Setting $J = J_{L/R}$ with $J_{L/R}/J_c \gg 1$ and $\gamma = 0$, the side chains act as wideband gapless reservoirs with $h = h_{L/R}$. In the following, we set $h_L = -h_R = \Delta h$ and work in units where $J_c = 1$. Employing a Jordan-Wigner mapping, this model can be transformed into a set of noninteracting spinless fermions. Following our wideband treatment for the reservoirs (i.e., $J_{L/R}/J_c \to \infty$), we obtain that $\Gamma_{L/R} \propto J'^2/J_{L/R}$ are the hybridization constants characterizing the contacts, with J' the couplings of the central region with the side chains, and $\mu_{L/R} = 2h_{L/R}$.

In the Markovian limit ($\Delta h \to \infty$) this model was shown to exhibit a steady-state phase transition where the decay of the correlators $C_{l,m} = \langle\sigma_l^z\sigma_m^z\rangle - \langle\sigma_l^z\rangle\langle\sigma_m^z\rangle$, as a function of $r = |l-m|$, passes from power law, for $h_c/J_c < 1-\gamma_c^2$, to exponential, for $h_c/J_c > 1-\gamma_c^2$ [8]. We address the non-Markovian regime (finite Δh) and monitor the steady-state energy current $\mathcal{J}_e$ and $f_{\rm nM}$ in addition to $C_{l,m}$ (explicit forms are given in the Supplemental Material). Figure 2(b) shows the

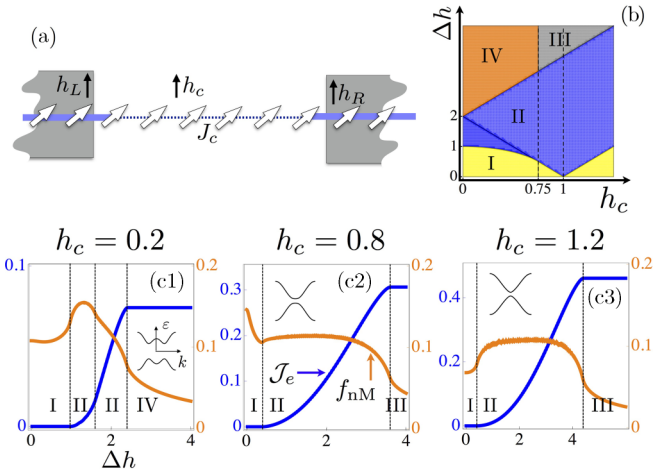

FIG. 2. (Color online) (a) Sketch of the XY model coupled to spin reservoirs with $T_L = T_R = 0$ and $h_L = -h_R = \Delta h$. (b) Phase diagram of the nonequilibrium steady state in the h_c-Δh plane computed for $\gamma_c = 0.5$, $J_c = 1$. Regions I–IV are described in the text. (c) Measurement of non-Markovianity $f_{\rm nM}$ and energy current $\mathcal{J}_e$ as a function of the spin imbalance Δh computed for different values of h_c and $\gamma_c = 0.5$. The band structures of the spinless Jordan-Wigner fermions are depicted in the insets.

phase diagram in the h_c-Δh plane and signals the four different steady-state phases. The energy current and $f_{\rm nM}$ as a function of Δh are given in Figs. 2(c1)–2(c3) for different values of h_c. A numerical analysis of the exponential/algebraic decay of $C_{l,m}$ within each region is provided in the Supplemental Material. In region I both effective chemical potentials ($\mu_{L/R}$) are below the excitation gap. This region shows a vanishing energy current and an exponential decay of $C_{l,m}$. In region II there is energy transport with a finite $d\mathcal{J}_e/d\Delta h$ and an algebraic decay of $C_{l,m}$. In this region $\mu_{R/L}$ lie within the excitation energy band. Regions III and IV show a saturation of the energy current and $f_{\rm nM}$ behaves as $1/\Delta h$ as the Markovian limit is taken. However, in region III, $C_{l,m}$ is algebraically decaying whereas in region IV the decay is exponential.

These results show that the two Markovian phases reported in Ref. [8] can be continuously connected to phases III and IV. Moreover, deep into the non-Markovian regime, phases I and II arise, having no Markovian analog.

Discussion. The explicit construction of the master equations for quadratic fermionic models coupled to wideband reservoirs permits the identification of the jump operators and decoherence rates derived from a microscopic Hamiltonian within the nonequilibrium Green's function formalism. The simplifications introduced by the wideband approximation greatly reduced the complexity of the equations of motion for the density matrix and allow one to treat extended systems. The approach permits one to characterize decoherence rates and to clarify the regimes where the Markovian limit yields a good approximation for the dynamics. Particular examples of non-Markonian evolution show how decoherence rates evolve as a function of time and how the Markovian limit can be reached as a function of the thermodynamic properties of the reservoirs. Our examples show that a set of nonequilibrium steady-state phases with distinct physical properties can be obtained upon changing the reservoir's properties. The method provides an explicit approach to study the real-time dynamics of a wide class of open systems.

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