Fate of dynamical phase transitions at finite temperatures and in open systems

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When a quantum system is quenched from its ground state, the time evolution can lead to nonanalytic behavior in the return rate at critical times t_c. Such *dynamical phase transitions* (DPTs) can occur, in particular, for quenches between phases with different topological properties in Gaussian models. In this paper we discuss Loschmidt echos generalized to density matrices and obtain results for quenches in closed Gaussian models at finite temperatures as well as for open-system dynamics described by a Lindblad master equation. While cusps in the return rate are always smoothed out by finite temperatures we show that dissipative dynamics can be fine-tuned such that DPTs persist.

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I. INTRODUCTION

The macroscopic properties of a quantum system in equilibrium can be understood from the appropriate thermodynamic potential. Studies of Lee-Yang zeros of the grand-canonical potential as a function of a complex fugacity or of Fisher zeros of the canonical potential as a function of complex temperature, in particular, have significantly contributed to our understanding of equilibrium phase transitions [1–4]. In recent years, there have been attempts to follow a similar approach to nonequilibrium dynamics. For quench dynamics in closed quantum systems it has been suggested that *dynamical phase transitions* (DPTs) can be defined based on the Loschmidt echo [5]

$$\mathcal{L}_0(t) = \langle\Psi_0|e^{-iH_1t}|\Psi_0\rangle. \tag{1.1}$$

Here $|\Psi_0\rangle$ is the pure quantum state before the quench and H_1 the time-independent Hamiltonian responsible for the unitary time evolution. The Loschmidt echo has the form of a partition function with boundaries fixed by the initial state. In analogy to the Fisher zeros in equilibrium one can thus study the zeros of the Loschmidt echo for complex time t. In Ref. [5] it has been shown that for the specific case of the transverse Ising model these zeros form lines in the complex plane which cross the real axis only for a quench across the equilibrium critical point.

In a many-body system one expects that the overlap between the time-evolved and the initial state is in general exponentially small in system size in analogy to the *Anderson orthogonality catastrophe* in equilibrium [6]. To obtain a nonzero and well-defined quantity in the thermodynamic limit it is thus useful to consider the return rate

$$l_0(t) = -\lim_{L\to\infty}\frac{1}{L}\ln|\mathcal{L}_0(t)|, \tag{1.2}$$

where L is the system size. Zeros in $\mathcal{L}_0(t)$ at critical times t_c then correspond to nonanalyticities (cusps or divergencies) in $l_0(t)$ [5,7–11]. It is, however, important to stress that in contrast to the particularly simple case of the transverse Ising model there is in general no one-to-one correspondence between dynamical and equilibrium phase transitions [8,12]. It is possible to find nonanalytical behavior of the return rate without crossing an equilibrium critical point in the quench, and one can cross a critical line without nonanalyticities in $l_0(t)$ being present. For one-dimensional topological systems it has been shown, in particular, that crossing a topological phase transition in the quench always leads to a DPT but the opposite does not have to be true [13]. Thus there are still some issues about the appropriateness of the Loschmidt echo as a useful indicator. Nevertheless the notion of a dynamical phase transition is an exciting concept extending key elements of many-body physics to nonequilibrium.

Lately, DPTs have also been studied experimentally. In Ref. [14] vortices in a gas of ultracold fermions in an optical lattice were studied and their number interpreted as a dynamical order parameter which changes at a DPT. Even more closely related to the described formalism to classify DPTs is an experiment where a long-range transverse Ising model was realized with trapped ions. In this case the time-evolved state was projected onto the initial state which allowed access to the Loschmidt echo (1.1) directly [15].

While these experiments are an exciting first step to test these far-from-equilibrium theoretical concepts, they also lead to a number of new questions. Chief among them is the question of how experimental imperfections affect the Loschmidt echo and DPTs. On the one hand, the initial state is typically not a pure state but rather is a mixed state at a certain temperature T. This raises the question how the Loschmidt echo can be generalized to thermal states. On the other hand, the dynamics is also typically not purely unitary. Decoherence and particle loss processes do affect the dynamics as well, requiring a generalization of (1.1) to density matrices. Finally dynamical

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processes and phase transitions can be induced entirely by coupling to reservoirs in which case no pure-state or $T = 0$ limit exists [16].

In this paper we address these questions. In Sec. II we discuss various different ways to generalize the Loschmidt echo to finite temperatures. We concentrate, in particular, on projective measurements of time-evolved density matrices relevant, for example, for trapped ion experiments, as well as on a proper distance measure between the initial and the time-evolved density matrix following Refs. [17,18]. We study both of these generalized Loschmidt echos for the case of unitary dynamics of Gaussian fermionic models in Sec. III. As examples, we present results for the transverse Ising and for the Su-Schrieffer-Heeger (SSH) model. In Sec. IV we consider the generalized Loschmidt echo for open-system dynamics of Gaussian fermionic models described by a Lindblad master equation (LME). A short summary and conclusions are presented in Sec. V.

II. THE LOSCHMIDT ECHO

We first review some properties of the standard Loschmidt echo for unitary dynamics of pure states in Sec. II A before discussing several possible generalizations to mixed states in Sec. II B.

A. Pure states

The Loschmidt echo for unitary dynamics of a pure state is defined by Eq. (1.1). Its absolute value can be used to define a metric in Hilbert space $\phi = \arccos|\mathcal{L}_0(t)|$, with $0 \leqslant |\mathcal{L}_0(t)| \leqslant 1$, which characterizes the distance between the initial state $|\Psi_0\rangle$ and the time-evolved state $|\Psi(t)\rangle = e^{-iH_1t}|\Psi_0\rangle$ [19]. From this point of view the Loschmidt echo is a time-dependent version of the *fidelity* $F = |\langle\Psi_0|\Psi_1\rangle|$ which has been widely used to study equilibrium phase transitions [17,20–33]. Because of the Anderson orthogonality catastrophe one has to consider the fidelity density $f = -\lim_{L\to\infty}\ln|F|/L$ for a many-body system in the thermodynamic limit $L \to \infty$ in analogy to the Loschmidt return rate defined in Eq. (1.2). If $|\Psi_0\rangle$ and $|\Psi_1\rangle$ are both ground states of a Hamiltonian $H(\lambda)$ for different parameters λ then the fidelity susceptibility $\chi_f = (\partial^2 f)/(\partial\lambda)^2|_{\lambda=\lambda_c}$ will typically diverge at an equilibrium phase transition. Similarly, one might expect that a quench can lead to states $|\Psi(t_c)\rangle$ at critical times t_c which are orthogonal to the initial state implying $\mathcal{L}_0(t_c) = 0$ and resulting in a nonanalyticity in the return rate $l_0(t_c)$. A peculiarity of the return rate is that its nonanalyticity depends not only on the properties of the initial and final Hamiltonian before and after the quench but also on time. For a quench from H_0 to H_1, in particular, the critical time t_c will in general depend upon if one starts with the ground state of the initial Hamiltonian or some excited eigenstate.

B. Mixed states

1. Loschmidt echo as a metric

If the Loschmidt echo is primarily seen as defining a metric in Hilbert space, then it is natural to ask if a similar metric can also be defined for density matrices $\rho(t)$. In order for the generalized Loschmidt echo $|\mathcal{L}_\rho[\rho(0),\rho(t)]|$ to give rise to a proper measure of distance in the space of density matrices we want the following relations to hold:

(i) $0 \leqslant |\mathcal{L}_\rho[\rho(0),\rho(t)]| \leqslant 1$ and $|\mathcal{L}_\rho[\rho(0),\rho(0)]| = 1$,
(ii) $|\mathcal{L}_\rho[\rho(0),\rho(t)]| = 1$ iff $\rho(0) = \rho(t)$, and
(iii) $|\mathcal{L}_\rho[\rho(0),\rho(t)]| = |\mathcal{L}_\rho[\rho(t),\rho(0)]|$.

Without time dependence, this problem reduces again to the definition of a fidelity for density matrices [34–36]. A direct generalization of this fidelity leads to [17,18]

$$\mathcal{L}_\rho(t) \equiv |\mathcal{L}_\rho[\rho(0),\rho(t)]| = \mathrm{Tr}\sqrt{\sqrt{\rho(0)}\rho(t)\sqrt{\rho(0)}}. \quad (2.1)$$

Note that this definition satisfies $\lim_{\beta\to\infty}\mathcal{L}_\rho(t) = |\mathcal{L}_0(t)|$ if $\rho(0)$ is a thermal density matrix and the time evolution is unitary. $\beta = T^{-1}$ is the inverse temperature with $k_B = 1$. $\mathcal{L}_\rho(t)$ is symmetric between $\rho(0)$ and $\rho(t)$ and also satisfies the other conditions above. The induced metric $\phi = \arccos[\mathcal{L}_\rho(t)]$ also fulfills the triangle inequality [19]. From this point of view, Eq. (2.1) is thus the proper generalization of the Loschmidt echo to density matrices. Despite its relatively complicated appearance, $|\mathcal{L}_\rho(\rho_1,\rho_2)|$ has a straightforward physical meaning [36]. If we understand ρ_1 and ρ_2 as reduced density matrices obtained by a partial trace over a larger system which is in a pure state $|\phi_{1,2}\rangle$, respectively, then $|\mathcal{L}_\rho(\rho_1,\rho_2)| = \max|\langle\phi_1|\phi_2\rangle|$ where the maximum is taken over all purifications of ρ_1 and ρ_2, respectively. That is, $\mathcal{L}_\rho$ provides the purification to the states in the enlarged Hilbert space which are as parallel as possible and consistent with the mixed states of the subsystem.

A seemingly simpler and more straightforward generalization such as

$$|\tilde{\mathcal{L}}_\rho(t)| = \sqrt{\frac{\mathrm{Tr}\{\rho(0)\rho(t)\}}{\mathrm{Tr}\,\rho^2(0)}} \quad (2.2)$$

does, in general, not fulfill the conditions above. If we start, for example, in a completely mixed state $\rho(0) = \sum_n \frac{1}{N}|\Psi_n\rangle\langle\Psi_n|$ and evolve under dissipative dynamics to a pure state $\rho(t\to\infty) = |\Psi_0\rangle\langle\Psi_0|$, then $|\tilde{\mathcal{L}}_\rho(0)| = |\tilde{\mathcal{L}}_\rho(\infty)| = 1$, which clearly is not a desirable property. Using a spectral representation in a basis where $\rho(0) = \sum_n p_n|\Psi_n^0\rangle\langle\Psi_n^0|$ is diagonal, Eq. (2.2) for the special case of unitary time evolution can be represented as

$$|\tilde{\mathcal{L}}_\rho(t)|^2 = \frac{\sum_{m,n} p_m p_n \left|\langle\Psi_m^0|e^{-iHt}|\Psi_n^0\rangle\right|^2}{\sum_n p_n^2}, \quad (2.3)$$

where p_n are weights with $\sum_n p_n = 1$.

In Sec. III we investigate $\mathcal{L}_\rho(t)$ for unitary dynamics in Gaussian models with $\rho(0)$ being a canonical density matrix at a given finite temperature T. At the same time, we also briefly discuss the result for $\tilde{\mathcal{L}}_\rho(t)$ which—for unitary dynamics—in this specific case does fulfill $0 \leqslant |\tilde{\mathcal{L}}_\rho(t)| \leqslant 1$. This is no longer the case for open-system dynamics described by an LME and we therefore exclusively discuss $\mathcal{L}_\rho(t)$ in Sec. IV.

2. Projection onto a pure state

While (2.1) allows one to generalize the properties of the Loschmidt echo as a metric to density matrices, $\mathcal{L}_\rho(t)$ might not necessarily be the quantity measured experimentally. In Ref. [15], for example, DPTs in the transverse Ising model have been investigated using a system of trapped ions. In this experiment the system is prepared in an initial configuration; the system is then time evolved and the Loschmidt echo measured by a projection. If the system is prepared in a pure state and the projection is onto the same pure state, then the Loschmidt echo (1.1) is measured. Here we want to consider the case that the preparation of the system is not ideal—leading to a mixed instead of a pure state—while the projection is still onto the ground state of the initial Hamiltonian. That is, we consider the case that only one of the states is impure. In this case we can define a generalized Loschmidt echo by replacing $\rho(0) \to |\Psi_0^0\rangle\langle\Psi_0^0|$ in Eq. (2.1), leading to

$$\begin{aligned} |\mathcal{L}_p(t)|^2 &= \langle\Psi_0^0|\rho(t)|\Psi_0^0\rangle/\langle\Psi_0^0|\rho(0)|\Psi_0^0\rangle \\ &= \sum_n \frac{p_n}{p_0}|\langle\Psi_0^0|e^{-iHt}|\Psi_n^0\rangle|^2. \end{aligned} \tag{2.4}$$

The second line is a spectral representation in the eigenbasis of $\rho(0)$ and we have introduced a normalization factor such that $\mathcal{L}_p(0) = 1$. Note that for a thermal initial density matrix $\lim_{\beta\to\infty}|\mathcal{L}_p(t)|^2 = |\mathcal{L}_0(t)|^2$. In Sec. III we also investigate this generalization of the Loschmidt echo for unitary dynamics and present results for experimentally relevant cases such as the transverse Ising model and the SSH model.

3. Alternative generalizations

The definition of a generalized Loschmidt echo for mixed states is not unique and several other possible generalizations have been discussed previously in the literature. In Refs. [37,38] the quantity

$$\mathcal{L}_{\text{av}} = \text{Tr}\{\rho(0)U(t)\} = \sum_n p_n\langle\Psi_n^0|e^{-iH_1t}|\Psi_n^0\rangle \tag{2.5}$$

is considered where $U(t)$ is the time-evolution operator. From the spectral representation for unitary time evolution with a time-independent Hamiltonian shown in the second line of Eq. (2.5) it is clear that this generalization measures an average over pure-state Loschmidt echos rather than the "overlap" between mixed states as defined in Eq. (2.1). Also in contrast to (2.3) only diagonal terms enter; Eq. (2.5) cannot be used to define a measure of distance between *two* density matrices. For a generic Gibbs ensemble one expects, in general, that $\mathcal{L}_{\text{av}} = 0$ is only possible if $p_0 = 1$, since even if the Loschmidt echos of different states $|\Psi_n^0\rangle$ will vanish at some time, the corresponding critcial times will in general be different. For a Gaussian model in a *generalized Gibbs ensemble*, where the occupation of each k mode is individually conserved, zeros are however also possible at finite temperatures [38].

A similar approach—motivated by the characteristic function of work [39]—was also used in Ref. [40] where the specific case of a canonical density matrix as the initial condition was considered and a generalized Loschmidt echo was defined by

$$\begin{aligned} \tilde{\mathcal{L}}_{\text{av}} &= \frac{1}{Z}\text{Tr}\{e^{iH_1t}e^{-iH_0t}e^{-\beta H_0}\} \\ &= \frac{1}{Z}\sum_n e^{-(\beta+it)E_n^0}\langle\Psi_n^0|e^{iH_1t}|\Psi_n^0\rangle. \end{aligned} \tag{2.6}$$

The result is a thermal average over the Loschmidt echo of pure states and thus is very different from the overlap between density matrices defined in Eq. (2.1).

For all generalized Loschmidt echos discussed here an appropriate return rate (1.2) can be defined. It is the return rate in the thermodynamic limit which we want to study in the following.

III. UNITARY DYNAMICS IN GAUSSIAN MODELS

We consider free fermion models described by the Hamiltonian

$$H = \sum_{k\geqslant 0}\Psi_k^\dagger\mathcal{H}_k\Psi_k, \tag{3.1}$$

with $\Psi_k = (c_k, c_{-k}^\dagger)^T$. Here c_k is an annihilation operator of spinless fermions with momentum k. This Hamiltonian describes models with a single-site unit cell which are bilinear in the creation and annihilation operators and can contain pairing terms as in the transverse Ising and Kitaev chains [see Sec. III B 1]. If we identify $d_k \equiv c_{-k}^\dagger$ then the Hamiltonian (3.1) can also describe models with a two-site unit cell which contain only hopping terms and no pairing terms such as in the SSH and Rice-Mele models [see Sec. III B 2]. The momentum summation in both cases runs over the first Brillouin zone. It is often convenient to write the 2×2 matrix $\mathcal{H}_k$ as $\mathcal{H}_k = \mathbf{d}_k\cdot\sigma$, where $\mathbf{d}_k$ is a three-component parameter vector and σ the vector of Pauli matrices. During the quench the parameter vector $\mathbf{d}_k$ is changed, leading to an initial Hamiltonian H_0 and a final Hamiltonian H_1. In the two different bases in which the Hamiltonians are diagonal we have

$$H_i = \sum_{k\geqslant 0}\varepsilon_k^i(c_{ki}^\dagger c_{ki} + c_{-ki}^\dagger c_{-ki} - 1), \tag{3.2}$$

with energies $\varepsilon_k^i > 0$ and $i = 0,1$. The operators in which the two Hamiltonians are diagonal are related by a Bogoliubov transform:

$$c_{k0} = u_k c_{k1} + v_k c_{-k1}^\dagger;\quad c_{k1} = u_k c_{k0} - v_k c_{-k0}^\dagger. \tag{3.3}$$

The Bogoliubov variables can be parametrized by an angle θ_k as $u_k = \cos\theta_k$ and $v_k = \sin\theta_k$. For each k mode there are four basis states. We can either work in the eigenbasis $|\Psi_j^0\rangle$ of H_0 or the eigenbasis $|\Psi_j^1\rangle$ of H_1, which can be expressed as

$$\begin{aligned} |\Psi_0^0\rangle &= |0\rangle_0 = (u_k - v_k c_{k1}^\dagger c_{-k1}^\dagger)|0\rangle_1, \\ |\Psi_1^0\rangle &= c_{k0}^\dagger|0\rangle_0 = c_{k1}^\dagger|0\rangle_1, \\ |\Psi_2^0\rangle &= c_{-k0}^\dagger|0\rangle_0 = c_{-k1}^\dagger|0\rangle_1, \\ |\Psi_3^0\rangle &= c_{k0}^\dagger c_{-k0}^\dagger|0\rangle_0 = (v_k + u_k c_{k1}^\dagger c_{-k1}^\dagger)|0\rangle_1, \end{aligned} \tag{3.4}$$

or vice versa

$$\begin{aligned} |\Psi_0^1\rangle &= |0\rangle_1 = (u_k + v_k c_{k0}^\dagger c_{-k0}^\dagger)|0\rangle_0, \\ |\Psi_1^1\rangle &= c_{k1}^\dagger|0\rangle_1 = c_{k0}^\dagger|0\rangle_0, \\ |\Psi_2^1\rangle &= c_{-k1}^\dagger|0\rangle_1 = c_{-k0}^\dagger|0\rangle_0, \\ |\Psi_3^1\rangle &= c_{k1}^\dagger c_{-k1}^\dagger|0\rangle_1 = (-v_k + u_k c_{k0}^\dagger c_{-k0}^\dagger)|0\rangle_0. \end{aligned} \tag{3.5}$$

Here $|0\rangle_{0,1}$ are the ground states of $H_{0,1}$. The Loschmidt echo at zero temperature can be easily calculated using the transformation (3.4), leading to

$$\mathcal{L}_0(t) = \prod_k \left[u_k^2 e^{i\varepsilon_k^1 t} + v_k^2 e^{-i\varepsilon_k^1 t}\right] = \prod_k \left[\cos\left(\varepsilon_k^1 t\right) + i\sin(2\theta_k)\sin\left(\varepsilon_k^1 t\right)\right] \tag{3.6}$$

and $|\mathcal{L}_0(t)|^2 = \prod_k |\mathcal{L}_0^k(t)|^2$, with

$$\left|\mathcal{L}_0^k(t)\right|^2 = \left[1 - \sin^2(2\theta_k)\sin^2\left(\varepsilon_k^1 t\right)\right]. \tag{3.7}$$

Here $\cos(2\theta_k) = \hat{\mathbf{d}}_k^0 \cdot \hat{\mathbf{d}}_k^1$ with $\hat{\mathbf{d}}_k^i$ being the normalized parameter vector. Note that the result (3.6) is also valid for free fermion models with a two-site unit cell but without pairing terms, although the ground state is different. From (3.7) it is evident that $\mathcal{L}_0(t_c) = 0$ if a momentum k_c exists with $\hat{\mathbf{d}}_{k_c}^0 \cdot \hat{\mathbf{d}}_{k_c}^1 = 0$, i.e., $\sin(2\theta_k) = 1$. The critical times are then given by

$$t_c = \frac{\pi}{2\varepsilon_{k_c}^1}(2n+1). \tag{3.8}$$

For any of the generalized Loschmidt echos defined before we can write the return rate as

$$l(t) = -\frac{1}{2\pi}\int \ln|L^k(t)|dk. \tag{3.9}$$

In the following we explicitly calculate $l(t)$ for the different generalized Loschmidt echos.

A. Projection onto a pure state

We want to first investigate the case where only one of the states is impure. A natural generalization is then the Loschmidt echo defined in Eq. (2.4). For the considered Gaussian models (3.1) the Loschmidt echo separates into the product $|\mathcal{L}_p(t)|^2 = \prod_k |\mathcal{L}_p^k(t)|^2$. If we, furthermore, assume that our initial mixed state is described by a canonical ensemble then we obtain

$$\left|\mathcal{L}_p^k(t)\right|^2 = \langle\Psi_0^0|\rho_k(t)|\Psi_0^0\rangle/\langle\Psi_0^0|\rho_k(0)|\Psi_0^0\rangle = \sum_{n=0}^{3} e^{-\beta(E_{kn}^0 - E_{k0}^0)}\left|\langle\Psi_0^0|e^{-iH_1 t}|\Psi_n^0\rangle\right|^2, \tag{3.10}$$

where we have used the spectral representation of the density matrix $\rho_k(t)$ in terms of the eigenstates of $\mathcal{H}_k^0$ and β is the inverse temperature. The eigenenergies of the four eigenstates for each k mode are denoted by $E_{kn}^0 = (-\varepsilon_k^0, 0, 0, \varepsilon_k^0)$. Using the representation (3.4) of the eigenstates in terms of the operators of the final Hamiltonian H_1 one finds

$$|\mathcal{L}_p(t)|^2 = \prod_k \left[1 - \left(1 - e^{-2\beta\varepsilon_k^0}\right)\sin^2(2\theta_k)\sin^2\left(\varepsilon_k^1 t\right)\right]. \tag{3.11}$$

It is obvious that $\mathcal{L}_p(t) = 0$ is only possible at zero temperature, in which case $|\mathcal{L}_p(t)| \equiv |\mathcal{L}_0(t)|$ [see Eq. (3.7)]. If one starts from a mixed state then the DPTs are washed out even if one projects onto the ground state. With the appropriately chosen ground state and the associated energies E_{kn}^0, the result (3.11) also holds for the models with a two-site unit cell such as in the SSH and Rice-Mele models.

B. Thermal density matrices

The calculation of (2.1) for the case that $\rho(0)$ is a thermal density matrix is instructive for the dissipative case discussed in Sec. IV so we briefly rederive the known result [17,18] for $\mathcal{L}_\rho(t)$ here. It is most convenient to perform the calculation in the eigenbasis of the time-evolving Hamiltonian H_1 using the transformation (3.5). Because only the states $|\Psi_0^i\rangle$ and $|\Psi_3^i\rangle$ are mixed by the transformation, the initial unnormalized density matrix $\rho_k(0)$ can be rearranged into two 2×2 block matrices $\mathbf{I}_2$ (identity matrix) and $\mathbf{r}_k(0)$, with

$$\boldsymbol{r}_k(0) = \begin{pmatrix} \cosh\left(\beta\varepsilon_k^0\right) + \sinh\left(\beta\varepsilon_k^0\right)\cos(2\theta_k) & -\sinh\left(\beta\varepsilon_k^0\right)\sin(2\theta_k) \\ -\sinh\left(\beta\varepsilon_k^0\right)\sin(2\theta_k) & \cosh\left(\beta\varepsilon_k^0\right) - \sinh\left(\beta\varepsilon_k^0\right)\cos(2\theta_k) \end{pmatrix}. \tag{3.12}$$

$\sqrt{r_k(0)}$ is obtained from (3.12) by replacing $\beta \to \beta/2$ and $r_k(t)$ by replacing $r_k^{(12)} \to e^{2i\varepsilon_k^1 t} r_k^{(12)}$ and $r_k^{(21)} \to e^{-2i\varepsilon_k^1 t} r_k^{(21)}$. The partition function is given by $Z_k = \mathrm{Tr}\,\rho_k = \mathrm{Tr}(\mathbf{I}_2) + \mathrm{Tr}\,\mathbf{r}_k(0) = 2 + 2\cosh(\beta\varepsilon_k^0)$. We can now simplify the generalized Loschmidt echo (2.1) in this case to

$$\mathcal{L}_\rho(t) = \prod_k \frac{2 + \lambda_{k1}(t) + \lambda_{k2}(t)}{2 + 2\cosh\left(\beta\varepsilon_k^0\right)}, \tag{3.13}$$

where $\lambda_{ki}^2(t)$ are the eigenvalues of $\sqrt{\mathbf{r}_k(0)}\mathbf{r}_k(t)\sqrt{\mathbf{r}_k(0)}$, which are given by

$$\lambda_{k1,2}(t) = \sqrt{1 + \left|\mathcal{L}_0^k(t)\right|^2 \sinh^2\left[\beta\epsilon_k^0\right]} \pm \left|\mathcal{L}_0^k(t)\right|\sinh\left[\beta\epsilon_k^0\right], \tag{3.14}$$

with $\mathcal{L}_0^k(t)$ defined in Eq. (3.7). As a final result we thus obtain [17,18]

$$\mathcal{L}_\rho(t) = \prod_k \frac{1 + \sqrt{1 + \left|\mathcal{L}_0^k(t)\right|^2 \sinh^2\left(\beta\varepsilon_k^0\right)}}{1 + \cosh\left(\beta\varepsilon_k^0\right)}. \tag{3.15}$$

For any finite temperature this means that $\mathcal{L}_\rho(t) > 0$ for all times; i.e., there are no DPTs. For $\beta \to \infty$ the result reduces to the zero-temperature result, Eq. (3.7). The result (3.15) also holds for Gaussian models with a two-site unit cell such as in the SSH and Rice-Mele models.

We now also briefly discuss the possible generalization $\tilde{\mathcal{L}}_\rho(t)$ defined in Eq. (2.2). While this function, in general, does not fulfill the requirements listed in Sec. II B, it turns out that for the case considered here at least $0 \leqslant |\tilde{\mathcal{L}}_\rho(t)| \leqslant 1$ is fulfilled. We start again from a thermal density matrix. The spectral representation using the eigenstates of H_1

then reads

$$|\tilde{\mathcal{L}}_\rho(t)|^2 = \frac{\sum_{n,m} e^{i(E_m^1 - E_n^1)t} \left|\langle \Psi_n^1 | e^{-\beta H_0} | \Psi_m^1 \rangle\right|^2}{\sum_n e^{-2\beta E_n^0}}. \tag{3.16}$$

Only the eigenstates $|\Psi_0^1\rangle$ and $|\Psi_3^1\rangle$ mix and it is easy to check the final result:

$$\begin{aligned} |\tilde{\mathcal{L}}_\rho(t)|^2 &= \prod_k \left[\cosh^{-2}\left(\beta\varepsilon_k^0\right) + \tanh^2\left(\beta\varepsilon_k^0\right) |\mathcal{L}_0^k(t)|^2 \right] \\ &= \prod_k \left[1 - \tanh^2\left(\beta\varepsilon_k^0\right) \sin^2(2\theta_k) \sin^2\left(\varepsilon_k^1 t\right)\right]. \end{aligned} \tag{3.17}$$

$\tilde{\mathcal{L}}_\rho(t) = 0$ is again only possible if $T = 0$.

1. Ising and Kitaev models

The finite-temperature results can be directly applied to concrete models. The Kitaev chain, for example, is defined by

$$H = \sum_i [\Psi_i^\dagger (\Delta i \boldsymbol{\tau}^y - J \boldsymbol{\tau}^z) \Psi_{i+1} + \text{H.c.} - \Psi_i^\dagger \mu \boldsymbol{\tau}^z \Psi_i], \tag{3.18}$$

where $\Psi_i^\dagger = (c_i^\dagger, c_i)$ and $c_i^{(\dagger)}$ annihilates (creates) a spinless particle at site i. The Kitaev chain is topologically nontrivial when $\mu < 2|J|$ and $\Delta \neq 0$. Note that $\Delta = 0$ is a phase boundary between phases with winding numbers ± 1. As a special case the transverse Ising model

$$H(g) = -\frac{1}{2} \sum_i \boldsymbol{\sigma}_i^z \boldsymbol{\sigma}_{i+1}^z + \frac{g}{2} \sum_{i=1}^N \boldsymbol{\sigma}_i^x \tag{3.19}$$

is obtained if one sets $\mu = -g/2$ and $J = 1/4 = -\Delta$ in (3.18). After a Fourier transform, for a chain with periodic boundary conditions, the Hamiltonian (3.18) is of the form of Eq. (3.1) with the parameter vector

$$\mathbf{d}_k = \left(0, 2\Delta \sin k, -2J \cos k - \mu\right), \tag{3.20}$$

and $\cos(2\theta_k) = \hat{\mathbf{d}}_k^0 \cdot \hat{\mathbf{d}}_k^1$. In Fig. 1 we plot the return rate in the thermodynamic limit, Eq. (3.9), for a quench in the transverse Ising model from $g = 0.5$ to $g = 1.5$.

While the cusp in the return rate at the critical time t_c is only slightly rounded off for temperatures up to $T = 0.1$ if we project onto the ground state, Eq. (2.4), signatures of a DPT are already almost lost at this temperature if we use the generalized Loschmidt echo (2.1) which measures the distance between the initial and the time-evolved thermal density matrix.

2. SSH and Rice-Mele models

The Rice-Mele and the SSH chains are models with a two-site unit cell and alternating hoppings $1 \pm \delta$ and potentials $\pm V$. The Hamiltonian for the Rice-Mele model is given by

$$\begin{aligned} H = &\sum_i \Psi_i^\dagger [-(1+\delta)\boldsymbol{\sigma}^x + V\boldsymbol{\sigma}^z] \Psi_i \\ &- (1-\delta) \sum_j \Psi_i^\dagger \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \Psi_{i+1} + \text{H.c.}, \end{aligned} \tag{3.21}$$

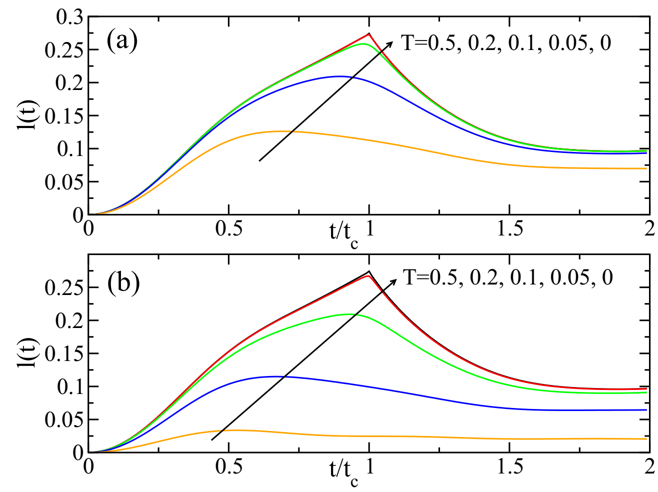

FIG. 1. The return rate $l(t)$ for the Ising chain in the thermodynamic limit for a quench from $g = 0.5$ to $g = 1.5$ at different temperatures T. (a) Projection onto the ground state, Eq. (3.11) (note that the curves for $T = 0$ and $T = 0.05$ are almost on top of each other). (b) Generalized Loschmidt echo, Eqs. (2.1) and (3.15).

with $\Psi_i = (c_i, d_i)$. After a Fourier transform this model can also be represented by the generic Hamiltonian (3.1) with the identification $d_k \equiv c_{-k}^\dagger$. The parameter vector in this case is given by

$$\mathbf{d}_k = (-2\cos k, 2\delta \sin k, V). \tag{3.22}$$

The SSH model is a special case of the Rice-Mele model obtained by setting the alternating potential $V = 0$.

In Fig. 2 the return rate for a symmetric quench from $\delta = -0.5$ to $\delta = 0.5$ for $V = 0$ is shown. While the cusp in the return rate at the critical time t_c is washed out in this case as well, a signature of the DPT at zero temperature is more clearly visible also at finite temperatures as compared to the quench in the Ising model shown in Fig. 1.

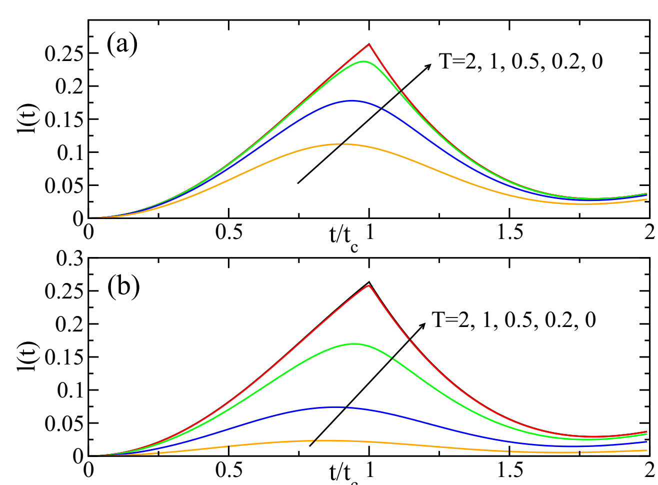

FIG. 2. The return rate $l(t)$ for the SSH chain in the thermodynamic limit for a quench from $\delta = -0.5$ to $\delta = 0.5$ at different temperatures T. (a) Projection onto the ground state, Eq. (3.11). (b) Generalized Loschmidt echo, Eq. (3.15). Note that the curves for $T = 0$ and $T = 0.2$ are almost on top of each other.

IV. OPEN SYSTEMS

In systems where the Loschmidt echo has been studied experimentally, such as cold atomic gases and trapped ions [14,15], interactions with electromagnetic fields are used to control the particles. These systems are therefore intrinsically open systems and decoherence and loss processes are unavoidable. Using the Born-Markov approximation such open systems can be described by a Lindblad master equation:

$$\dot{\rho}(t) = -i[H,\rho] + \sum_\mu \left(L_\mu \rho L_\mu^\dagger - \frac{1}{2}\{L_\mu^\dagger L_\mu,\rho\}\right). \quad (4.1)$$

Here L_μ are the Lindblad operators describing the dissipative, nonunitary dynamics induced by independent reservoirs labeled by μ, and $\{\cdot,\cdot\}$ is the anticommutator. In order to have a bilinear LME which can be solved exactly, we continue to consider Hamiltonians as defined in Eq. (3.1) with periodic boundary conditions which can be diagonalized in Fourier space. We consider Lindblad operators that are linear in creation and annihilation operators, leading to the linear dynamics

$$L_\mu = \sqrt{\gamma_\mu} c_\mu \quad \text{and} \quad L_\mu = \sqrt{\bar{\gamma}_\mu} c_\mu^\dagger \quad (4.2)$$

describing particle loss and creation processes with amplitudes $\gamma_\mu > 0$ and $\bar{\gamma}_\mu > 0$, respectively. This form ensures that the dissipative terms in Eq. (4.1) are also bilinear. More specifically we consider reservoirs that couple each to only one k mode:

$$L_k = \sqrt{\gamma_{\pm k}} c_{\pm k} \quad \text{and} \quad L_k = \sqrt{\bar{\gamma}_{\pm k}} c_{\pm k}^\dagger. \quad (4.3)$$

To solve the Lindblad equation we use the superoperator formalism [41]. The $n \times n$ density matrix ρ is recast into an n^2-dimensional vector $||\rho\rangle\rangle$ and the Hamiltonian and Lindblad operators become superoperators acting on this vector. The LME (4.1) and its solution can then be written as

$$||\dot{\rho}\rangle\rangle = \mathcal{L}\,||\rho\rangle\rangle; \quad ||\rho\rangle\rangle(t) = \exp(\mathcal{L}t)\,||\rho(0)\rangle\rangle. \quad (4.4)$$

For the purely unitary time evolution considered in the previous section the Lindbladian $\mathcal{L}$ takes the form

$$\mathcal{L} = -i(H \otimes \mathbf{I}_n + \mathbf{I}_n \otimes H^\dagger), \quad (4.5)$$

where $\mathbf{I}_n$ is the $n \times n$ identity matrix. Similarly, the individual Lindblad operators (4.3) can be written as superoperators acting on $||\rho\rangle\rangle$. The solution vector $||\rho\rangle\rangle(t)$ can then be recast into a matrix allowing one to calculate the generalized Loschmidt echos also for open systems.

A. Particle loss

We consider again free fermionic models of the type (3.1) with the four basis states (3.4) for each k mode.

As a first example, we investigate the simple mixed initial state $\rho_k(0) = \frac{1}{2}(|\Psi_1^0\rangle\langle\Psi_1^0| + |\Psi_2^0\rangle\langle\Psi_2^0|)$ and a time evolution under the Lindblad operators $L_{1k} = \sqrt{\gamma_k} c_k$ and $L_{2k} = \sqrt{\gamma_{-k}} c_{-k}$. In this case it is straightforward to show that the density matrix takes the form $\rho_k(t) = \frac{1}{2}\text{diag}(2 - e^{-\gamma_k t} - e^{-\gamma_{-k} t}, e^{-\gamma_k t}, e^{-\gamma_{-k} t}, 0)$. The nonequilibrium steady state (NESS) is thus the completely empty state for $\gamma_{\pm k} \neq 0$. Since both $\rho(0)$ and $\rho(t)$ are diagonal it follows immediately that the generalized Loschmidt echo is given by

$$\mathcal{L}_\rho(t) = \frac{1}{2}\prod_k (e^{-\gamma_k t/2} + e^{-\gamma_{-k} t/2}). \quad (4.6)$$

As one might have expected, $\mathcal{L}_\rho(t)$ shows an exponential decay in this case. If $\gamma_k = \gamma_{-k} = \gamma =$ const then the return rate in the thermodynamic limit (3.9) increases linearly, $l(t) = \gamma t/2$, and thus diverges only at infinite time.

B. Quench in Kitaev-type models with particle loss

Next, we want to consider a quench for a Kitaev-type model with Hamiltonian (3.2) with the basis states (3.5). As in Sec. III B we start with the thermal density matrix $\rho(0)$ but now also allow for particle loss processes as in the example above. Crucially, the matrix $\rho_k(t)$ still can be decomposed into two 2×2 block matrices. We can therefore write $\mathcal{L}_\rho^k(t) = \text{Tr}\sqrt{M_1} + \text{Tr}\sqrt{M_2}$, with $M_i = \sqrt{\rho_k^i(0)}\rho_k^i(t)\sqrt{\rho_k^i(0)}$ and $\rho_k^{1,2}$ being the two block matrices. With $\text{Tr}\sqrt{M_i} = \sqrt{\lambda_1^i} + \sqrt{\lambda_2^i} > 0$ we can write $(\text{Tr}\sqrt{M_i})^2 = \lambda_1^i + \lambda_2^i + 2\sqrt{\lambda_1^i\lambda_2^i} = \text{Tr}\, M_i + 2\sqrt{\det M_1}$ [36]. For the Loschmidt echo we therefore find

$$\mathcal{L}_\rho(t) = \prod_k \sum_{i=1,2} \sqrt{\text{Tr}\, M_i + 2\sqrt{\det M_i}}\,. \quad (4.7)$$

Using this formula it is straightforward to obtain an explicit result for $\mathcal{L}_\rho(t)$ which, however, is quite lengthy for finite temperatures. We therefore limit ourselves here to presenting the result for $T = 0$ only. In this case one of the block matrices is zero and we obtain the following closed-form expression

$$L_\rho^2(t) = \prod_k e^{-\Gamma_k^+ t}\Big\{\cos 2\theta_k \sinh(\Gamma_k^+ t) - \sin^2 2\theta_k \sin^2(\varepsilon_k^1 t) + \frac{1}{2}\sin^2 2\theta_k\big[1 - \cosh(\Gamma_k^- t)\big] + \cosh(\Gamma_k^+ t)\Big\}. \quad (4.8)$$

Here we have defined $\Gamma_k^\pm = (\gamma_k \pm \gamma_{-k})/2$. It is easy to see that this result reduces to Eq. (3.7) for $\gamma_k = \gamma_{-k} = 0$. Furthermore, there are no DPTs for finite loss rates.

As an example for the broadening of the cusps in the return rate (3.9) we consider the same quench in the transverse Ising model as before.

Figure 3 shows that small loss rates already lead to a significant broadening of the first cusp at $t = t_c$ and completely wash out the cusps at longer times. Furthermore, the NESS for a nonzero loss rate is always the empty state, so that the return rate at infinite times becomes *independent* of the loss rate and is given by

$$l(t \to \infty) = -\frac{1}{2\pi}\int_0^\pi \ln\left(\frac{1 + \hat{\mathbf{d}}_k^0 \cdot \hat{\mathbf{d}}_k^1}{2}\right) dk. \quad (4.9)$$

C. Quench in Kitaev-type models with particle creation and loss

So far we have seen that both finite temperatures and particle loss processes destroy DPTs. One can then ask if it is possible to engineer dissipative processes in an open quantum system in such a way that DPTs persist. By constructing a concrete example we show that this is indeed possible.

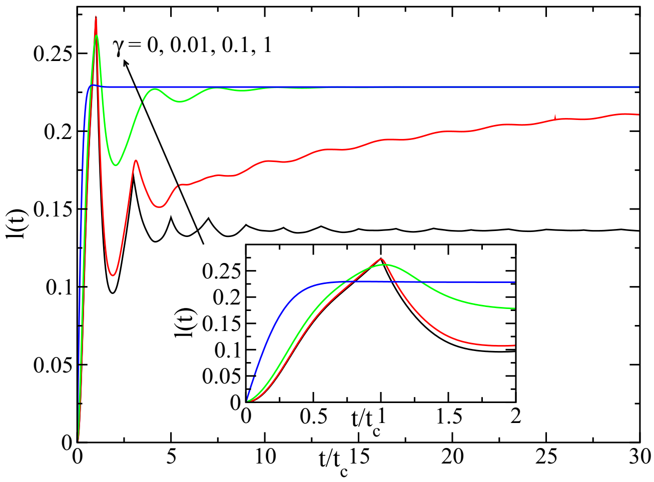

FIG. 3. The return rate $l(t)$ for the Ising chain in the thermodynamic limit for a quench from $g = 0.5$ to $g = 1.5$ at $T = 0$ for different particle loss rates $\gamma = \gamma_k = \gamma_{-k}$. Inset: Broadening of the first cusp at $t = t_c$.

We consider the case that particles with momentum k are annihilated with rate γ_k while particles with momentum $-k$ are created with rate $\bar{\gamma}_{-k}$. As in the case with particle loss considered in Sec. IV B the density matrix $\rho_k(t)$ still has block structure, and a calculation along the same lines is possible. At $T = 0$ we obtain a result which is very similar to Eq. (4.8) and reads

$$L^2_\rho(t) = \prod_k e^{-\tilde{\Gamma}^+_k t}\bigg\{\cos 2\theta_k \sinh(\tilde{\Gamma}^-_k t) - \sin^2 2\theta_k \sin^2\left(\varepsilon^1_k t\right) + \frac{1}{2}\sin^2 2\theta_k[1-\cosh(\tilde{\Gamma}^-_k t)] + \cosh(\tilde{\Gamma}^-_k t)\bigg\}. \tag{4.10}$$

The rates are now defined as $\tilde{\Gamma}^\pm_k = (\gamma_k \pm \bar{\gamma}_{-k})/2$. The essential difference when comparing Eq. (4.10) with the previous result (4.8) is that inside the bracket only the rate $\tilde{\Gamma}^-_k$ is present. For $\tilde{\Gamma}^-_k = 0$, i.e., $\gamma_k = \bar{\gamma}_{-k}$, the Loschmidt echo becomes $L^2_\rho(t) = \prod_k \exp(-\tilde{\Gamma}^+_k t)|\mathcal{L}^k_0(t)|^2$, which is the zero-temperature result (3.7) with an additional exponential decay. DPTs are thus still present for this particular case at the same critical times t_c despite the dissipative processes.

As an example, we consider again the quench in the transverse Ising chain. In Fig. 4 we show results for the fine-tuned point $\gamma = \gamma_k = \bar{\gamma}_{-k}$. The cusps remain clearly visible for finite dissipation rates. For the k-independent rate $\tilde{\Gamma}^+_k \equiv \tilde{\Gamma}^+$ as chosen in Fig. 4 the result for the return rate is

$$l(t) = \frac{\tilde{\Gamma}^+ t}{2} - \frac{1}{\pi}\int_0^\pi \ln\left|\mathcal{L}^k_0(t)\right| dk. \tag{4.11}$$

This is simply the zero-temperature return rate in the closed system plus a linear increase with slope $\tilde{\Gamma}^+/2$. In the NESS at long times all particles will be in the $-k$ states, leading to a vanishing Loschmidt echo and a diverging return rate.

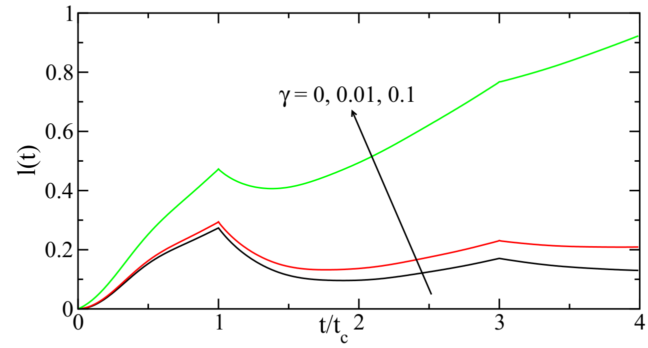

FIG. 4. The return rate $l(t)$ for the Ising chain in the thermodynamic limit for a quench from $g = 0.5$ to $g = 1.5$ at $T = 0$ for various equal particle loss and creation rates $\gamma = \gamma_k = \bar{\gamma}_{-k}$.

V. CONCLUSIONS

We have studied a generalization of the Loschmidt echo to density matrices which is applicable both to finite temperatures and to open systems. It is based on a direct generalization of the fidelity for mixed states to dynamical problems and provides a measure of the distance between the initial and the time-evolved density matrix. As such it is very different from previous generalizations studied in the context of dynamical phase transitions which are based on thermal averages over the Loschmidt echos of pure states and are only applicable to unitary dynamics.

For bilinear one-dimensional fermionic lattice models with periodic boundary conditions we have shown that finite temperatures always wash out the nonanalyticities in the return rate of the generalized Loschmidt echo. Dynamical phase transitions only exist at zero temperature.

For open quantum systems described by a Lindblad master equation we similarly find that particle loss processes smooth out cusps in the return rate so that signatures of the dynamical phase transition are hard to detect even if the loss rates are very small.

Finally, we showed that it is possible to fine-tune particle loss and creation processes in such a way that dynamical phase transitions can be observed despite the dissipative dynamics.

The generalized Loschmidt considered in this paper can be understood as a tool to measure distances between density matrices. As such it might be helpful in engineering and controlling specific states using dissipative dynamics. Zeros of the Loschmidt echo signal, in particular, that a mixed state has been reached such that all purifications to states in an enlarged Hilbert space are orthogonal to purifications of the initial state.

Note added. Recently Ref. [42] became available, which is on a related topic.

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