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# Disentangling dynamical phase transitions from equilibrium phase transitions

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Dynamical phase transitions (DPTs) occur after quenching some global parameters in quantum systems, and are signalled by the nonanalytical time evolution of the dynamical free energy, which is calculated from the Loschmidt overlap between the initial and time evolved states. In a recent Letter [M. Heyl *et al.*, Phys. Rev. Lett. **110**, 135704 (2013)], it was suggested that DPTs are closely related to equilibrium phase transitions (EPTs) for the transverse field Ising model. By studying a minimal model, the *XY* chain in a transverse magnetic field, we show analytically that this connection does not hold generally. We present examples where DPT occurs without crossing any equilibrium critical lines by the quench, and a nontrivial example with no DPT but crossing a critical line by the quench. Although the nonanalyticities of the dynamical free energy on the real time axis do not indicate the presence or absence of an EPT, the structure of Fisher lines for complex times reveals a qualitative difference.

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Interest in nonequilibrium dynamics has grown immensely in the past few years [1–4] thanks to experimental advances made with ultracold atomic gases. The wide controllability of these systems allows experimentalists to prepare different kinds of nonequilibrium initial states and it is also possible to study the dynamics with time resolution that is unreachable in other physical systems [5–9]. Some of the main questions concern when and how thermalization, or more generally, equilibration, occurs and its connection to ergodicity and integrability. These were first posed by von Neumann in 1929 [10].

The nonequilibrium time evolution can be characterized in many different ways, borrowing ideas from equilibrium statistical mechanics. The ultrashort time nonequilibrium dynamics, revealing the role of high-energy excitations, is also of interest as well as the stationary state that is reached after long time evolution. The latter can be described by the diagonal ensemble, which is roughly the time averaged density matrix. The results of local measurements can be described by simpler ensembles, i.e., by the thermal Gibbs ensemble for nonintegrable (ergodic) systems [11] and by the generalized Gibbs ensemble for integrable ones [12]. The Loschmidt overlap (LO), which is the main focus of this Rapid Communication, is a nonlocal expression and is entirely determined by the diagonal ensemble, hence it characterizes the stationary state [13]. Analyzing the LO has proven to be useful in studying quantum chaos, decoherence, and quantum criticality [14–17]. It is defined as the scalar product of the initial state and the time evolved state following a sudden global quench (SQ) as

$$G(t) = \langle\psi|e^{-iHt}|\psi\rangle, \tag{1}$$

and can be regarded as the characteristic function of work performed on the system during the quench. In a SQ the parameters of the Hamiltonian are changed suddenly from some initial to final values, and the system, prepared initially in the ground state $|\psi\rangle$ of the initial Hamiltonian, is assumed to be well separated from the environment and evolves unitarily with $H$.

In a recent Letter, Heyl *et al.* [18] pointed out a similarity between the time evolution of the LO overlap and the equilibrium phase transitions (EPTs). Close to phase transitions the free energy density is a nonanalytical function of the temperature. A method proposed by Fisher [19] to analyze the zeros of the partition function in the *complex temperature plane* gives a good understanding of these nonanalyticities. In a finite system phase transitions cannot occur, and the Fisher zeros are isolated and do not lie on the real axis. However, in the thermodynamic limit they coalesce into lines (or, in a general case, areas [20]) that can cross the real axis. These crossings are responsible for the breakdown of the analytic continuation of the free energy density as a function of temperature: Knowing the free energy above the transition temperature does not give any information about the free energy below.

The LO in Eq. (1) is formally similar to the canonical partition function with imaginary temperature. For a large system $G(t)$ scales exponentially with the system size, and hence it is worthwhile to study the dynamical free energy [13,21], which we define as

$$f(t) = -\lim_{N\to\infty}\frac{1}{N}\ln G(t). \tag{2}$$

Under certain circumstances this quantity shows nonanalytical time evolution. Due to the similarities with the EPT, the notion *dynamical phase transitions* (DPTs) were introduced in Ref. [18]. It was found that in the transverse field Ising chain the DPTs and EPTs are ultimately related: The time evolution of $G(t)$ becomes nonanalytic whenever the magnetic field is quenched through the (equilibrium) critical value. Similar observations were made for nonintegrable models [22] and for complex magnetic fields [23].

The purpose of this Rapid Communication is to show that this connection is not rigorous. To this aim we investigate the anisotropic *XY* chain in a transverse magnetic field and show that generally DPTs can occur in quenches within the same phase, i.e., without crossing any equilibrium phase boundary. Note that numerical evidence for this phenomenon was reported recently in Refs. [13,24]. In addition, we also present a counterexample where the quench crosses an equilibrium critical point, but the LO remains analytic.

The *XY* Hamiltonian with periodic boundary conditions reads as

$$H(\gamma,h) = \sum_{j=1}^{N} \frac{1+\gamma}{2}\sigma_j^x\sigma_{j+1}^x + \frac{1-\gamma}{2}\sigma_j^y\sigma_{j+1}^y - h\sigma_j^z, \quad (3)$$

where $\gamma$ and $h$ are the anisotropy parameter and the homogeneous external magnetic field, respectively. This model can be mapped to free fermions with the use of the Jordan-Wigner transformation as

$$H(\gamma,h) = \sum_{j=1}^{N-1} c_j^+c_{j+1} + \gamma c_j^+c_{j+1}^+ - h\left(c_j^+c_j - \frac{1}{2}\right) + \text{H.c.}$$
$$-\mu(c_N^+c_1 + \gamma c_N^+c_1^+ + \text{H.c.}), \quad (4)$$

where $c_j$ are fermionic operators and $\mu = e^{i\pi N_f}$, $N_f = \sum_{i=1}^{N} c_i^+c_i$. This Hamiltonian conserves the parity of the particle number and acts differently on the even and odd subspaces (sometimes referred to as Neveu-Schwarz or Ramond sectors). The Hamiltonians in the two subspaces are formally the same if we impose an antiperiodic boundary condition for the even and periodic boundary condition for the odd subspace. In wave-number space these boundary conditions translate to different quantizations of the wave numbers, $k = \frac{2\pi}{N}(n+\frac{1}{2})$ in the even and $k = \frac{2\pi}{N}n$ in the odd subspace. In the fermionic language the ground state is unique in a given subspace, but when $|h| < 1$, the ground states with even and odd parity become degenerate in the thermodynamic limit. These parity eigenstates are the symmetric or antisymmetric combinations of the fully polarized states, and they do not possess magnetization in the coupling direction. We start our investigation with the parity eigenstates and we discuss polarized ground states in the Supplemental Material [25].

The LO is calculated analytically in both of the even ($e$) and odd ($o$) subspaces as

$$G_s(t) = e^{i\varphi_s(t)} \prod_{0<k<\pi} [\cos(\varepsilon_k t) + i\cos(2\Theta_k)\sin(\varepsilon_k t)], \quad (5)$$

where $\Theta_k = \theta_k^1 - \theta_k^0$ is the difference between the Bogoliubov angles diagonalizing the prequench ($\alpha = 0$) and postquench ($\alpha = 1$) Hamiltonians, $\varepsilon_k \equiv \varepsilon_k^1$ and for $s = o,e$, $\varepsilon_k^\alpha = 2\sqrt{[\cos(k) - h^\alpha]^2 + [\gamma^\alpha \sin(k)]^2}$. The Bogoliubov angles are determined from $e^{i2\theta_k^\alpha} = 2[\cos(k) - h^\alpha - i\gamma^\alpha\sin(k)]/\varepsilon_k^\alpha$, and the wave numbers are quantized with respect to the parity of the initial state. The phase factor satisfies $\varphi_e(t) = 0$ and $\varphi_o(t) = t(\pm\varepsilon_0 \pm \varepsilon_\pi)/2$, where the signs depend on the position of the initial and final Hamiltonian on the phase diagram [25].

We focus on the real part of the dynamical free energy, which is the same in the thermodynamic limit for both sectors. The nonanalytical behavior of the dynamical free energy is encoded in the zeros of the partition function $G(t)$ in the complex time plane [18]. Instead, following the practice in the literature, we determine these zeros in the complex "temperature" plane, i.e., the zeros of $Z(z) = \langle\psi|e^{-zH}|\psi\rangle = G(-it)$. Especially in the *XY* model, the Fisher zeros from $Z(z) = 0$ determine the dynamical free energy *completely* [25]. From Eq. (5), the Fisher zeros in the thermodynamic limit form lines indexed by an integer number $n$ as

$$z_n(k) = \frac{i\pi}{\varepsilon_k}\left(n + \frac{1}{2}\right) - \frac{1}{\varepsilon_k}\,\text{arth}[\cos(2\Theta_k)], \quad (6)$$

which agrees formally with Ref. [18], but in our case, the Bogoliubov angles depend on more variables, hence are a more general function of $k$. This increased freedom leads to interesting behavior of the Fisher lines. The main quantity that determines the dynamical free energy is $\cos(2\Theta_k)$, which can be expressed analytically with the parameters of the initial and final Hamiltonian. Furthermore, $\cos(2\Theta_k) = 1 - 2n_k$, where $n_k$ is the expectation value of the quasiparticle occupation number in the postquench Hamiltonian and is conserved under the time evolution. A Fisher line crosses the imaginary axis whenever $n_k = 1/2$, which can be interpreted as modes with infinite effective temperature. These crossings are responsible for the nonanalytic time evolution of the dynamical free energy.

Due to the parity of the cosine function it is evident that if a Fisher line crosses the imaginary axis for a quench $(h_0,\gamma_0) \to (h_1,\gamma_1)$, it implies a crossing in the reversed protocol $(h_1,\gamma_1) \to (h_0,\gamma_0)$ as well. We call this the symmetric property of DPT. This seems to be plausible in quenches crossing critical points, but it is less trivial for quenches within the same phase.

The phase diagram of the *XY* chain is drawn in Fig. 1. The excitation spectrum is gapless when $h = \pm 1$ or when $\gamma = 0$, $|h| < 1$. The Fisher lines, and hence the LO, show different behavior for quenching between different regions in the phase diagram. The exact values of the initial and final parameters $h_0$, $\gamma_0$, $h_1$, and $\gamma_1$ in given phases do not modify qualitatively the behavior of the LO as a sign of some kind of universality. We consider four types of quenches, where three of them can be realized by quenching one parameter only, while in third example one needs to quench both the magnetic field and the anisotropy parameter.

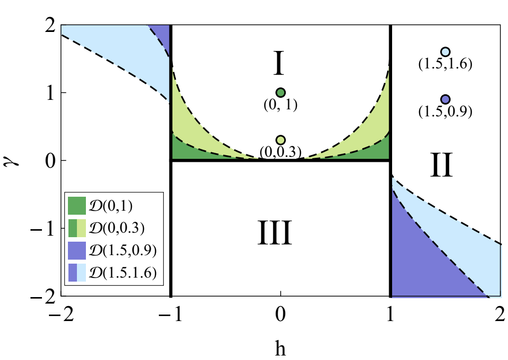


FIG. 1. (Color online) The phase diagram of the *XY* model in a magnetic field. The three studied phases (I, II, III) are marked on the plot. These gapless phases are separated by critical lines that form an H letterlike shape. DPTs can occur in quenches within the same phase. The domains $\mathscr{D}(h_0,\gamma_0)$ of the final parameters where DPTs appear are shown for four given initial conditions $(h_0,\gamma_0)$. Except from the region $h_1 < -1$, the domains are determined from Eq. (7). Note that when quenching from II to $h_1 < -1$, nonanalyticities only show up in the top left corner of the phase diagram and remain absent otherwise, in spite of crossing several critical lines.

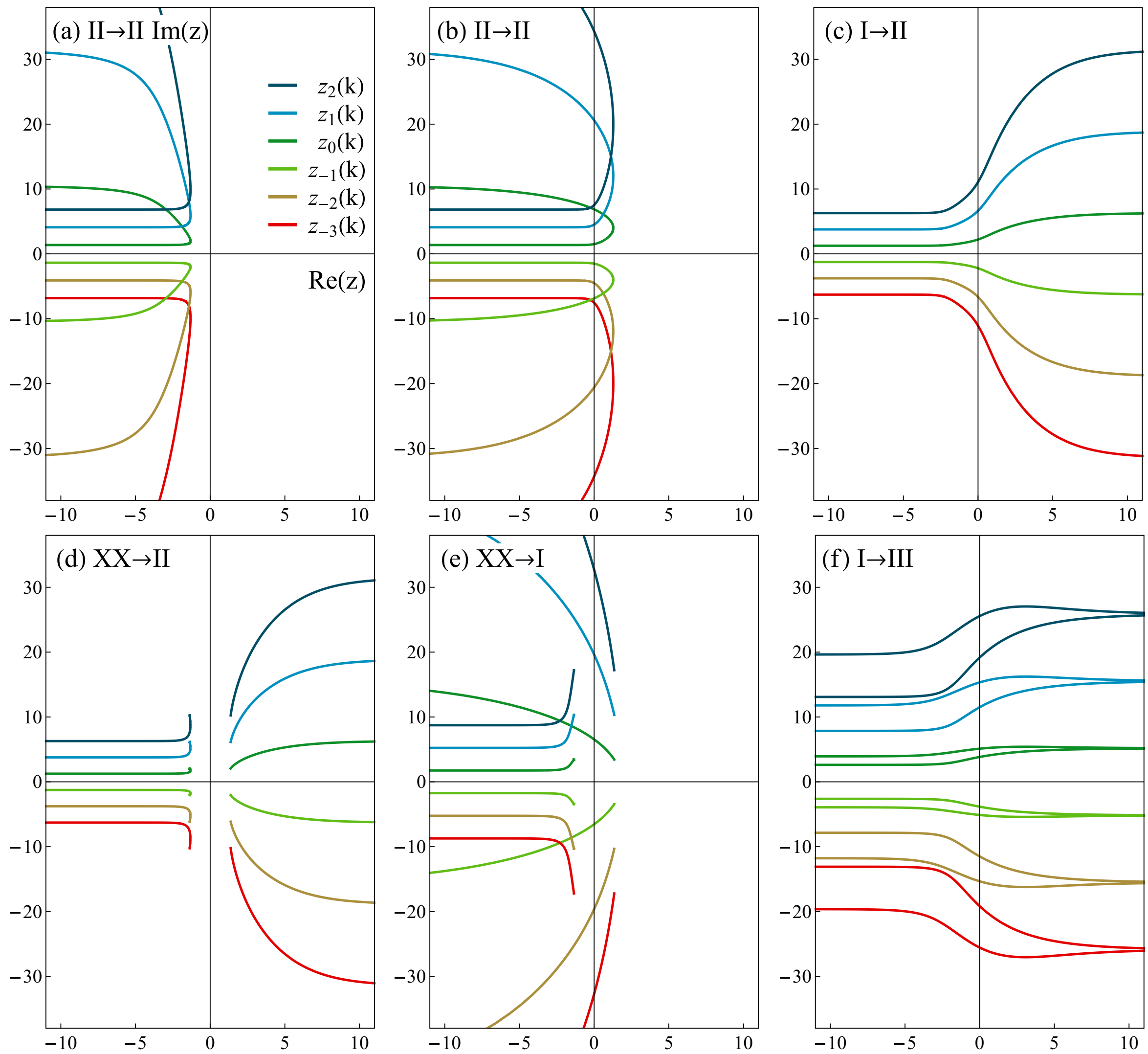


FIG. 2. (Color online) The flow of Fisher lines $z_n(k)$ [$n = (-3,\dots,2)$] for various types of quenches discussed in the main text.

*DPT without EPT: Quenches not crossing critical points.* We start our discussion with quenches inside phase II, where $h_{0,1} > 1$, and we assume that $\gamma_0 > 0$ without loss of generality. In this setup no critical lines are crossed by the parameters of the Hamiltonian during the quench, but DPTs can occur. Generally one can show that the $k \to 0,\pi$ tails of the Fisher lines lie in the left half plane: $\lim_{k\to 0} \mathrm{Re}\{z_n(k)\} = -\infty$ and $\lim_{k\to\pi} \mathrm{Re}\{z_n(k)\} = -\infty$. For small quenches all lines lie in the left half plane [Fig. 2(a)], hence the time evolution of the dynamical free energy is analytical. However, the turning point of the Fisher lines can move to the right half plane [Fig. 2(b)]. In this case each Fisher line crosses the time axis twice at wave numbers $k_1^*$ and $k_2^*$. The nonanalytical times are given by $t_i^* = \frac{\pi}{\varepsilon_{k_i^*}}(n + \frac{1}{2})$, $i = 1,2$. This occurs if the anisotropy parameter is quenched to a sufficiently negative value at a fixed magnetic field. No matter how $\gamma$ is quenched, an equilibrium critical point is never approached, but DPT shows up.

More generally, for each point $(h_0,\gamma_0)$ in phase II, the domain $\mathscr{D}(h_0,\gamma_0) \subset$ II of $(h_1,\gamma_1)$ where DPT occurs is given by

$$\mathscr{D}(h_0,\gamma_0)=\left\{(h_1,\gamma_1)|2\gamma_0\gamma_1 < 1-h_0h_1-\sqrt{\left(h_0^2-1\right)\left(h_1^2-1\right)}\right\} \quad (7)$$

within phase II. The boundary of these regions is a second order curve (a cone section). A few examples for these domains are shown in Fig. 1.

A similar phenomenon can be observed in quenches inside phase I. The Fisher lines start and end in the left half of the complex plane, but some parts of the lines can move to the right half plane. Given $(h_0,\gamma_0)$ in phase I, the domain of the final parameters where the nonanalyticities occur is given by Eq. (7) within phase I. For example, starting from the Ising model ($\gamma_0 = 1$, $h_0 = 0$), one needs to quench the magnetic field and the anisotropy parameter as well to see the nonanalytic behavior (see Fig. 1). However, considering smaller anisotropy, the DPT can appear by quenching solely the magnetic field when $\gamma_0 < \sqrt{1+|h_0|}/\sqrt{2}$ is satisfied for the initial Hamiltonian.

*DPT together with EPT: Quench between phases I and II*. In this setup the quenched parameters cross at least one critical point, and the time evolution of the dynamical free energy is always nonanalytical. The asymptotic behavior of the Bogoliubov angles guarantees that the Fisher lines cross the imaginary axis, that is, $\lim_{k\to 0}\mathrm{Re}\{z_n(k)\} = \infty$ and $\lim_{k\to\pi}\mathrm{Re}\{z_n(k)\} = -\infty$ [Fig. 2(c)]. Because of the symmetries of the $XY$ model, quenches between phase II and III behave in the same way.

*EPT without DPT: Quench from phase II to the critical XX line ($\gamma = 0, |h| < 1$)*. In quenches II $\to$ I,III, DPTs showed up everywhere except for quenches from phase II to the boundary of I and III. Though the asymptotic behavior of the Bogoliubov angles is similar to the I $\to$ II case, there is an interesting difference as well: There are no Fisher zeros in the vicinity of the imaginary axis. The function $\cos(2\Theta_k)$ is not continuous at $\tilde{k} = \arccos(\frac{h_1\gamma_0 - h_0\gamma_1}{\gamma_0-\gamma_1})$, therefore $\lim_{\varepsilon\to 0^+}\cos(2\Theta_{\tilde{k}\mp\varepsilon}) \lessgtr 0$. Hence the Fisher lines split into two sections that do not cross the imaginary axis [Fig. 2(d)].

By considering the $XX$ line as the $\gamma_1 \to 0$ limit, then as we approach the $XX$ line, the slope of $\cos(2\Theta_k)$ diverges at $\tilde{k}$, hence the density of the Fisher zeros vanishes near the imaginary axis. As opposed to previous examples, when the initial and final Hamiltonians did lie in the gapped phase, quenching to the $XX$ line is a special case because the final parameters are on a critical line. Nevertheless, it is still surprising that for quenches II $\to$ I,III DPTs occur everywhere except for the boundary of these regions.

However, nonanalytical behavior in the dynamical free energy can be observed in quenches to the critical lines as well. One example is a quench from I or III to the $XX$ line: $(\gamma_0 \neq 0, |h_0| < 1) \to (\gamma_1 = 0, |h_1| < 1)$ with $h_1 \neq h_0$. In this case, one would think naively that the Fisher lines would cross the imaginary axis twice, similarly to quenches I $\to$ I and I $\to$ III, but one of the crossings does not manifest itself [Fig. 2(e)] in a similar manner, as it was discussed above. The other example, which we only mention here, is a quench crossing a critical line [26]: starting from III to the $h = 1$ critical boundary of I.

*Quench from phase I to III*. In this case the anisotropy parameter is quenched from positive to negative values in a low magnetic field ($-1 < h_{0,1} < 1$). The system goes through an anisotropy transition at $\gamma = 0$. At $\gamma > 0$ the ground state polarization is in the $x$, while at $\gamma < 0$ it is in the $y$ direction. For these quenches $\lim_{k\to 0,\pi}\mathrm{Re}\{z_n(k)\} = -\infty$, meaning that the Fisher lines start and end at the left half plane. However, there is a wave number $0 < \tilde{k} < \pi$ defined by $\cos(\tilde{k}) = \frac{h_1\gamma_0 - h_0\gamma_1}{\gamma_0-\gamma_1}$, for which $\cos(2\Theta_{\tilde{k}}) = -1$. This means that while $k$ goes through the interval $(0,\pi)$, the Fisher lines come from $\mathrm{Re}\{z\} = -\infty$, reach $\mathrm{Re}\{z\} = \infty$ at $\tilde{k}$, and finally go back to $\mathrm{Re}\{z\} = -\infty$ again [Fig. 2(f)]. Hence all the Fisher lines cross the imaginary axis twice, giving rise to two emergent time scales in the dynamical free energy [Fig. 3(a)]. This is the qualitative difference between the quenches I to II and I to III.

For EPTs, the nonanalyticity of the free energy is also imprinted in the nonanalytic behavior of other physical quantities, e.g., the order parameter or its susceptibility. A similar phenomenon is expected to occur for the DPTs as well [18]. For the $XY$ model, the equilibrium order parameter is the magnetization in the $XY$ plane. Therefore, we determined its absolute value for the nonequilibrium situation by a numerical evaluation of Pfaffians [27]. Whenever the Fisher line crosses the imaginary axis once, only a single emergent nonequilibrium time scale appears from the dynamical free energy, which matches exactly that of the magnetization. However, for quenches I $\to$ I and I $\to$ III, each Fisher line crosses the imaginary axis twice, which implies two nonequilibrium time scales. Only these two time scales and their higher harmonics [in Fig. 3(d)] appear in the dynamics of magnetization, though generally we were not able to express analytically the zeros of the magnetization by the nonanalytic time scales. However, in the I $\to$ III quench protocol when $\gamma_0$ and $\gamma_1$ are not too close to the $\gamma = 0$ critical line, the magnetization takes zero values in the vicinity of the Fisher times [Figs. 3(a) and 3(b)].

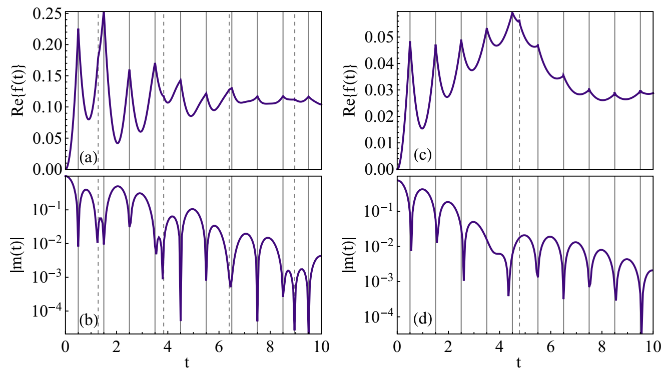


FIG. 3. (Color online) The dynamical free energy is nonanalytical at Fisher times $t_{i,n} = t_i^*(n + 1/2)$, $i = 1,2$ (solid and dashed lines, respectively). The time unit was chosen to be $t_1^*$. The longitudinal magnetization also shows two time scales: In (b) the zeros of the magnetization approximately lie at the Fisher times, and in (d) the relation between them is more involved. Quench parameters for (a) and (b) are $(h_0 = 0, \gamma_0 = 1) \to (h_1 = 0.6, \gamma_0 = -1)$ and for (c) and (d) they are $(h_0 = 0, \gamma_0 = 0.1) \to (h_1 = 0.6, \gamma_0 = 0.1)$.

Until now we considered quenches starting from even or odd parity eigenstates. It is an important question whether or not the nonanalytic behavior is present in quenches starting from polarized states. For quenches through the critical point in the transverse field Ising model it has been shown that DPTs can be observed, but the nonanalyticities are not at the Fisher times of the parity subspaces [18,22]. We found similar behavior in the $XY$ model [25].

Though we calculated the LO and the dynamical free energy directly from the time evolution of the initial wave function, they describe the stationary state after the quench [13]. That is, as the time evolution operator is diagonal in the eigenbasis of $H$, $G(t)$ depends only on the diagonal elements of the density matrix, $G(t) = \mathrm{Tr}\{\rho_{\mathrm{DE}}e^{-iHt}\}$, where $\rho_{\mathrm{DE}}$ is the diagonal ensemble. The diagonal density matrix depends on the fermion occupation numbers $n_k$ and it can be expressed explicitly [25],

$$\rho_{\mathrm{DE}} = \prod_{0<k<\pi}[n_k n_{-k} + \cos^2(\Theta_k)(1 - n_k - n_{-k})] \tag{8}$$

$$= \prod_{0<k<\pi}\cos^2(\Theta_k)\delta_{n_k,0}\delta_{n_{-k},0} + \sin^2(\Theta_k)\delta_{n_k,1}\delta_{n_{-k},1}. \tag{9}$$

From the latter form it is straightforward to reproduce Eq. (5). The correlation between wave numbers $k$ and $-k$ comes from the BCS superconductorlike initial state. The LO—up to a trivial phase factor—is the characteristic function of work done on the system [28], hence it depends on all moments of the energy. As it is a nonlocal quantity, the generalized Gibbs ensemble $\rho_{\mathrm{GGE}} \sim e^{\sum \lambda_k n_k}$, where $\lambda_k$ fixes the expectation value of $n_k$, would not give the proper result for the LO, because it does not describe well the correlations between $n_k$ and $n_{-k}$. With the diagonal ensemble in Eq. (8), we took into account the correlations among the modes, hence it can be applied to calculate any moment of the energy.

*Conclusion*. We analyzed the dynamical free energy for quenches in the *XY* model in a magnetic field. The singular behavior of the dynamical free energy is determined solely by the Bogoliubov angles through the quasiparticle occupation numbers and it is not sensitive to the spectra of the initial or final Hamiltonians. The appearance of DPTs is connected to the existence of modes with $1/2$ occupancy probability. In this particular system we explicitly demonstrated the existence of DPTs without an EPT as well as the absence of DPTs in the presence of EPTs. Though the dynamical free energy does not distinguish between DPTs with or without EPTs, the Fisher lines do. If the quench crosses a critical line, the Fisher lines sweep through the whole real axis. However, for quenches inside a given phase, the Fisher lines reach either $\infty$ or $-\infty$.

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[25] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevB.89.161105 for details about parity sectors, polarized states, density matrix, and determining Loschmidt overlap from Fisher lines.
[26] By this we mean that any curves connecting the initial and final parameters cross at least one critical line.
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