First-Order Dynamical Phase Transitions

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Recently, dynamical phase transitions have been identified based on the nonanalytic behavior of the Loschmidt echo in the thermodynamic limit [Heyl *et al.*, Phys. Rev. Lett. 110, 135704 (2013)]. By introducing conditional probability amplitudes, we show how dynamical phase transitions can be further classified, both mathematically, and potentially in experiment. This leads to the definition of first-order dynamical phase transitions. Furthermore, we develop a generalized Keldysh formalism which allows us to use nonequilibrium dynamical mean-field theory to study the Loschmidt echo and dynamical phase transitions in high-dimensional, nonintegrable models. We find dynamical phase transitions of first order in the Falicov-Kimball model and in the Hubbard model.

The last two decades have witnessed an extraordinary boost in the investigation of strongly correlated systems out of equilibrium, both experimentally and theoretically. This renewed interest is the consequence of the impressive experimental advances achieved in the manipulation of cold atoms in optical lattices [1–4], and in ultrafast time-resolved spectroscopy in solids [5–7]. Using systems of cold atoms, which are very well isolated from the environment and easily tunable, one can now address fundamental and long-standing problems in statistical physics. In particular, many intriguing phenomena have recently been uncovered in relation to the relaxation of excited many-body states towards thermal equilibrium [8]. Thermalization can be hampered due to (near) integrability [9] and delayed by prethermalization [10–12], and the different relaxation regimes can be separated by a narrow crossover as a function of some parameter [13,14]. Near symmetry-breaking phase transitions, the dynamics can be altered entirely by the presence of nonthermal critical points [15–17]. An unsolved question in this context is whether some of these dynamical crossover phenomena reflect an underlying "sharp" transition, involving a mathematical nonanalyticity of some nature.

In the transverse-field Ising model, Heyl *et al.* [18] found a nonanalytic time dependence of the Loschmidt echo, i.e., the probability to return to the initial state within a nontrivial time evolution. Although the latter is not directly related to the time dependence of thermodynamic observables, this observation suggests an intriguing new starting point for analyzing and classifying the dynamical behavior of many-particle systems. To be more precise, we consider a quantum quench, i.e., a sudden change of the Hamiltonian from some $H(t < 0) = H_0$ to $H(t \geq 0) = H$, which triggers a nontrivial out-of-equilibrium evolution. Heyl *et al.* [18] defined a dynamical phase transition (DPT) as a nonanalytic behavior of the return probability amplitude [19]

$$A(t) = \langle \psi_0 | e^{-iHt} | \psi_0 \rangle \qquad (1)$$

as a function of time, where $|\psi_0\rangle$ is the ground state of H_0. The return probability, defined by $L(t) \equiv |A(t)|^2$, is the Loschmidt echo. In analogy to the equilibrium partition function, which has a large deviation form $Z = \text{Tr} e^{-\beta H} \sim e^{-\beta N f(\beta)}$ in the thermodynamic limit $N \to \infty$ with a free energy density $f(\beta)$, $A(t)$ has a large deviation limit of the form $A(t) \sim e^{-Na(it)}$, and nonanalytic behavior as a function of time can occur in the thermodynamic limit [20].

Since the seminal work [18], further progress has been achieved in the understanding of DPTs [24–32], but important questions remain open. First, the Loschmidt echo is the probability of performing no work in a double quench experiment $H_0 \to H \to H_0$ [18], but it is not in any obvious, simple way related to the time evolution of physical observables, which also hampers a further characterization and classification of DPT's. Furthermore, DPTs may be hard to access in nonintegrable systems which do not allow for an exact solution: the computation of an overlap amplitude is most direct with wave-function based numerical techniques, which are, however, almost exclusively used for finite or one-dimensional systems. Examples thereof are exact diagonalization, which is restricted to small systems, or infinite DMRG [29]. In this Letter we present two concepts to address these questions: first we introduce conditional amplitudes and generalized expectation values, which allow for a further classification of DPTs and also for the definition of first-order transitions. Second, we explain how the amplitude (1) can be computed with diagrammatic many-body techniques and nonequilibrium dynamical mean-field theory [33], which makes it accessible for a large class of high-dimensional, interacting models directly in the thermodynamic limit.

First-order dynamical phase transitions.—As Eq. (1) gives the probability amplitude for the return to the initial state $|\psi_0\rangle$, a natural way to further classify a DPT is to more closely characterize the "path" along which this return happens. As we will see, a first-order DPT occurs when

these paths for infinitesimally different propagation times t can be distinguished by a nonvanishing change in a *macroscopic* measurement. To illustrate this idea, let $\hat{X} \equiv N\hat{x}$ be any observable which is extensive in the system size N. Then we can define a *conditional return amplitude*

$$\tilde{A}(t, x)\Delta x \equiv \langle\psi_0|e^{-iH(t-t_1)}\mathcal{P}_x^{\Delta x}e^{-iHt_1}|\psi_0\rangle, \quad (2)$$

where $\mathcal{P}_x^{\Delta x}$ can be any operator that selects eigenstates of $\hat{x}$ with eigenvalues in a small interval of size Δx around x, e.g., $\mathcal{P}_x^{\Delta x} \propto \sum_i e^{-[\langle i|\hat{x}|i\rangle-x]^2/2\Delta x^2}|i\rangle\langle i|$. (Note that this choice implies that $\mathcal{P}$, and, hence, $\tilde{A}(t, x)$ is a smooth function of x for finite systems.) In a many-body path integral formulation [34], Eq. (1) can be written as the sum over all paths in some configuration space (Grassmann variables for fermions, complex fields for bosons), with a boundary condition provided by the state $|\psi_0\rangle$, while $\tilde{A}(t, x)$ sums the subclass of paths fixed by the constraint $\hat{x} = x$ at the intermediate time $t = t_1$. By construction, we have $A(t) = \int dx \tilde{A}(t, x)$. Assuming again a large deviation form $\tilde{A}(t, x) = e^{-N\tilde{a}(it,x)}$ for $N \to \infty$, the integral will be dominated by its saddle-point values, i.e., $a(it) = \tilde{a}(it, x_*(t))$, where the complex number $x_*(t)$ is determined by $d\tilde{a}/dx|_{x=x_*} = 0$. In the presence of several saddle points the dominant one can change as a function of the parameter t, which defines a first-order dynamical transition, in analogy to first-order transitions in equilibrium. Because such a first-order transition is a change of the propagator (1), its detection should not depend on the particular choice of $\hat{x}$ or t_1, but should be reflected by an abrupt change of the generalized expectation value of a generic observable $\hat{Y}$,

$$\langle\hat{Y}(t_1)\rangle_A = A(t)^{-1}\langle\psi_0|e^{-iH(t-t_1)}\hat{Y}e^{-iHt_1}|\psi_0\rangle, \quad (3)$$

which is obtained from $A(t)$ by an infinitesimal variation $\langle\hat{Y}(t_1)\rangle_A = i(\delta\ln A_\eta(t)/\delta\eta(t_1))|_{\eta=0}$, of a field $\eta(t')$ coupling to $\hat{Y}$, with $A_\eta(t) = \langle\psi_0|T_t\exp[-i\int_0^t dt'(H + \eta(t')\hat{Y})]|\psi_0\rangle$. One of the main results of this work is that both the expectation values Eq. (3) and the rate $a(it)$ can be easily computed within the DMFT formalism, as we show later. It follows from the discussion above that the expectation value of $\hat{x}$ yields the complex saddle point $x_*(t)$, which abruptly changes as a function of t.

Before discussing first-order DPTs' in specific models, it is important to note how generalized expectation values are related to real measurements, in spite of the fact that the quantity $\langle\hat{Y}\rangle_A$ itself is in general complex and only real probabilities like the Loschmidt echo can be considered measurable. To make the connection, we consider the Loschmidt echo, $L_{\delta t}(t) \equiv |\langle\psi_0|e^{-iH(t-t_1)}e^{-ig\hat{Y}\delta t}e^{-iHt_1}|\psi_0\rangle|^2$ of an experiment with an extended quench protocol involving a quench $H_0 \to H$ at time zero, a short intermediate propagation from t_1 to $t_1 + \delta t$ with a Hamiltonian $g\hat{Y}$, and a final propagation with H [35]. Taking the limit of small δt yields

$$L_{\delta t}(t)/L(t) = 1 + 2g\delta t\,\mathrm{Im}\langle\hat{Y}\rangle_A + \mathcal{O}(g^2\delta t^2). \quad (4)$$

In essence, the intermediate propagation adds a phase kick to the propagator, thus measuring the imaginary part of $\langle\hat{Y}\rangle_A$.

Dynamical mean-field theory.—We now proceed to explain how the Loschmidt amplitude rate $a(it)$ and the expectation values (3) can be computed for high-dimensional fermionic lattice systems. In the study of quantum systems out of equilibrium, one of the most powerful techniques is dynamical mean-field theory (DMFT) [33,36], which captures local correlations in high-dimensional systems, by mapping a lattice model onto an effective impurity model. This mapping is exact in the limit of infinite dimensions [37]. Here we use it to study the generic correlated lattice model

$$H(t) = H_0 + U(t)\sum_i n_{i\uparrow}n_{i\downarrow}, \quad (5)$$

with $H_0 = -\sum_{\langle i,j\rangle\sigma}t_\sigma V_{ij}c_{i\sigma}^\dagger c_{j\sigma} + \mu\sum_{i\sigma}n_{i\sigma}$, which describes fermions with two (spin) flavors on a lattice: V_{ij} are lattice-dependent hoppings, t_σ is a spin-dependent prefactor of the hopping term, and $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$. The time-dependent local repulsion energy $U(t)$ is the parameter driving the sudden quench from H_0 to H: $U(t \le 0) = 0$ and $U(t > 0) = U$. The Hamiltonian (5) describes the Falicov-Kimball model when one spin flavor is localized ($t_\downarrow = 0$), and the Hubbard model when $t_\uparrow = t_\downarrow = 1$ (see below).

Nonequilibrium DMFT is based on the many-body Keldysh formalism, which is formulated in terms of Green's functions and thus does not directly give access to wave-function overlaps like in Eq. (1). In order to use a Green's function formalism to compute the overlap, we first introduce in Eq. (1) an identity $e^{-iH_0t}e^{iH_0t}$ and a fictitious temperature $1/\beta$, which is then sent to zero,

$$A(t) = \lim_{\beta\to\infty}e^{E_0(\beta-it)}\mathrm{Tr}(e^{-\beta H_0}e^{iH_0t}e^{-iHt}). \quad (6)$$

Formally, we can view the terms under the trace as the time ordering of a generalized contour-dependent Hamiltonian (GCH) defined on the Keldysh contour $\mathcal{C} = \mathcal{C}_1\cup\mathcal{C}_2\cup\mathcal{C}_3$,

$$\mathcal{Z}_\mathcal{C} \equiv \mathrm{Tr}(\mathcal{T}_\mathcal{C}e^{-i\int_\mathcal{C}dt'H_\mathcal{C}(t')}), \quad (7)$$

where the Hamiltonians $H_\mathcal{C}(t)$ on the upper ($\mathcal{C}_1$) and lower ($\mathcal{C}_2$) real branches are different, $H_\mathcal{C}(t) = H$ for $t \in \mathcal{C}_1$ and $H_\mathcal{C}(t) = H_0$ for $t \in \mathcal{C}_{2,3}$ (see Fig. 1). We can define contour-ordered expectation values $\langle\mathcal{O}\rangle_{H_\mathcal{C}} = \mathrm{Tr}[\mathcal{T}_\mathcal{C}e^{-i\int_\mathcal{C}dt'H_\mathcal{C}(t')}\mathcal{O}(t_1)]/\mathcal{Z}_\mathcal{C}$, which coincide with the generalized expectation values (3) in the limit $\beta \to \infty$.

At this point we note that the Keldysh formalism remains applicable when the Hamiltonian is an explicit function of the contour time. In particular, diagrammatic rules for contour-ordered Green's functions $G_{ij}(t_1, t_2) = -i\langle\mathcal{T}_\mathcal{C}c_i(t_1)c_j^\dagger(t_2)\rangle_{H_\mathcal{C}}$ remain unchanged, and one can
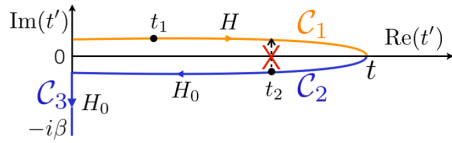
FIG. 1 (color online). Generalized contour-dependent Hamiltonian on the Keldysh contour $\mathcal{C}$. The upper, lower, and imaginary branches of the contour are denoted by $\mathcal{C}_1$, $\mathcal{C}_2$, and $\mathcal{C}_3$, respectively. The arrows indicate the contour ordering, in this case t_1 comes earlier than t_2, i.e., $t_1 \prec t_2$. For a Green function $G(t_1, t_2)$, if t_1 lies on $\mathcal{C}_1$ and t_2 lies on $\mathcal{C}_2$, the latter cannot be shifted to the upper contour.

define a self-energy and a Dyson equation formally identical to those for the standard contour Hamiltonian. With this, any argument leading to the DMFT formalism, based on either power counting or the cavity formalism [36] can be rewritten one to one for a generic contour dependence of $H_\mathcal{C}$. We use DMFT with GCHs to study the Falicov-Kimball and the Hubbard model, in the former using closed equations of motion, in the latter employing a quantum Monte Carlo algorithm [38]. Details on the DMFT solution and its implementation are given in the Supplemental Material [39].

Within the Green's function formalism, the overlap amplitude (6) is obtained from a coupling constant formalism. Taking the derivative of the free energy $a_U(it) = \lim_{N \to \infty} -(1/N) \ln A_U(t)$ involves the generalized expectation value of the double occupancy $d = (1/N)\sum_i n_{i\uparrow} n_{i\downarrow}$,

$$\frac{\partial a_U(it)}{\partial U} = -i \lim_{\beta \to \infty} \int_0^t dt' \langle d(t') \rangle_{H_\mathcal{C}(U)}, \qquad (8)$$

where the dependence of A [Eq. (6)] and $H_\mathcal{C}$ on the parameter U in H is made explicit. For convenience, we also define the integrated double occupation $\Delta(U,t) \equiv (1/t) \int_0^t dt' \langle d(t') \rangle_{H_\mathcal{C}(U)}$. The free energy is then just the integral of (8), i.e., $a(it) = \lim_{\beta \to \infty} it \int_0^U dU' \Delta(U', t)$.

Results.—As a first application of the above results, we focus on the Falicov-Kimball model (FKM). It describes two species of fermions: the itinerant ones, which can hop between neighboring sites, and the immobile ones, which act as an annealed disorder potential for the other species. The Hamiltonian is given by Eq. (5) with hopping $t_\sigma = 0$ for one species. The FKM can be solved exactly within DMFT [46]. It displays a rich phase diagram [47], including a paramagnetic metal-insulator transition at half-filling ($\langle n_\uparrow \rangle = \langle n_\downarrow \rangle = \frac{1}{2}$), which is located at $U_c = 2$ (independent of temperature) for the Bethe lattice. The possibility of an exact solution makes the FKM an important benchmark also for nonequilibrium DMFT [48–52], in spite of the peculiarity that thermalization is excluded because of the missing interaction between the itinerant fermions [50]. The DMFT equations for a GCH, which are analogous to the standard nonequilibrium DMFT solution [48], are given in the Supplemental Material [39].
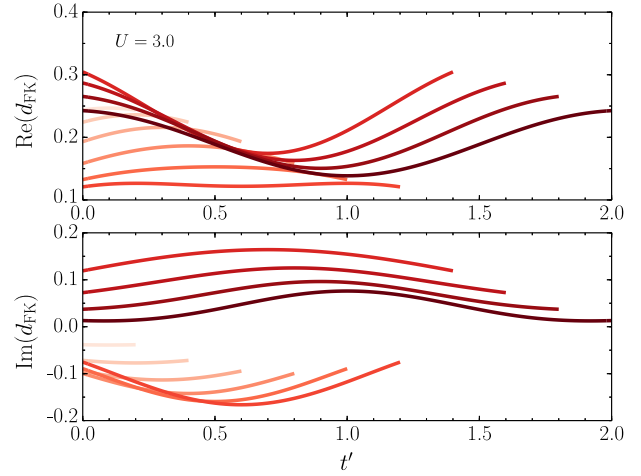

FIG. 2 (color online). Time-dependent generalized expectation value of the double occupancy $d_{FK}(t') \equiv \langle d(t') \rangle_{H_\mathcal{C}}$ in the FKM for $U = 3.0$ and increasing values of t from $t = 0.2$ to $t = 2.0$ (t is evident from the length of the contour, $0 \le t' \le t$). Upper panel: real part, lower panel: imaginary part. Data obtained with $\beta = 50$, a real-time discretization step $dt = 0.02$ and a mesh of $N_\tau = 200$ points on the imaginary axis (see the Supplemental Material [39] for technical details).

We will now show that the FKM undergoes a DPT. As can be seen in Fig. 2, our DMFT results indicate that the time-dependent generalized expectation value of the double occupation abruptly changes its shape with increasing t
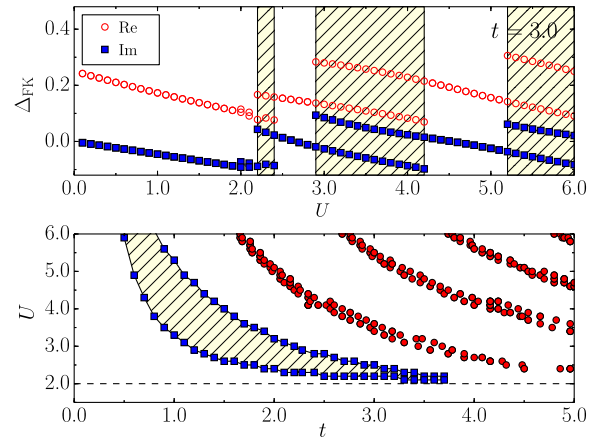

FIG. 3 (color online). Dynamical phase diagram of the FKM. Top: real and imaginary part of the integrated double occupation Δ_{FKM} obtained by increasing (decreasing) U in steps of $\Delta U = 0.1$ from $U = 0.1$ ($U = 6.0$), and using the solution at U as a seed for the iterative solution of DMFT at $U + \Delta U$ ($U - \Delta U$). Bottom: Blue squares show the coexistence region around the first transition branch, obtained at each t as described in the upper panel. For the other transition branches, we provide only lower-bound estimates for the coexistence region: In the region between red dots at the same t, two coexisting solutions are found by different choices in the update of the Green function at each DMFT iteration (see Supplemental Material [39]).
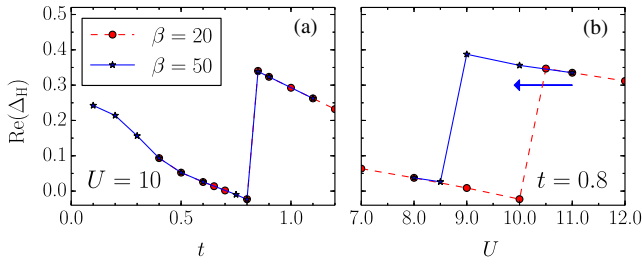
FIG. 4 (color online). DPT in the Hubbard model. Panel (a): Real part of the integrated double occupation for a quench to $U = 10$ at different t. To confirm the convergence of the results with the fictitious temperature, we show data for $\beta = 20$ (red circles) and $\beta = 50$ (blue stars). Panel (b): coexisting solutions for $\Delta_H(U)$ at $t = 0.8$ at different values of U. Red circles and blue stars are obtained using as an initial guess for the hybridization function in DMFT the noninteracting Green function on the Bethe lattice and the converged solution at $U = 11$, respectively.

(see, for example, the curves at $t = 1.2$ and 1.4). In the top panel of Fig. 3 we plot the integrated double occupancy $\Delta(U, t)$ as a function of U for given t. We indeed find a nonanalytic curve, which displays a sequence of jumps in whose vicinity two coexisting DMFT solutions for d_{FKM} are found. The coexistence of solutions evidences a *first-order* dynamical transition. We map out the coexistence region (shaded area in Fig. 3) by increasing (decreasing) U in small steps, using the solution at a given U as a starting input for the DMFT iteration at the next value of the interaction. In the lower panel of Fig. 3 blue squares give the bounds of the coexistence region obtained in this way, indicating a transition for quenches to all values $U > U_c$.

We have also applied our generalized Keldysh formalism to the Hubbard model, which describes correlated fermions with spin-$\frac{1}{2}$ on a lattice. A numerically exact solution of the nonequilibrium DMFT equations can be obtained with a continuous-time Monte Carlo impurity solver. The weak-coupling approach [38,53] allows us to simulate reasonably long time intervals, especially in the present setup, where the time evolution starts from a noninteracting equilibrium state, and where interaction vertices only have to be sampled on the forward branch $\mathcal{C}_1$. However, since the Green functions for GCHs lack causal symmetries [39], we cannot use the improved estimator introduced in Ref. [38], which makes the calculations time consuming.

Our results demonstrate that the Hubbard model also exhibits a first-order DPT. In Fig. 4(a) we show that the integrated double occupation after a quench in the strong coupling regime ($U = 10$) has a jump at $t \sim 0.85$. As in the case of the FKM, the first-order nature of the transition is signaled by a coexistence of solutions, as shown in Fig. 4(b). In contrast to the FKM, which is peculiar in the sense that even in equilibrium the metal-insulator transition prevails to all temperatures, the Hubbard model is a

nonintegrable model which does show thermalization after a quench [13].

Conclusions.—This Letter provides two main insights related to the study of DPTs. From a theoretical point of view, we have shown that dynamical phase transitions can be more deeply characterized by means of conditional probability amplitudes and generalized expectation values, which are experimentally accessible with suitable quench protocols. From a methodological point of view, our main result is that the Loschmidt echo can be obtained in the context of DMFT by considering a general contour-dependent Hamiltonian on the Keldysh contour. We find first-order DPTs both for the Falicov-Kimball and the Hubbard model. This raises the hope to actually observe DPT's in experiments with cold atoms, although issues like finite size effects and the influence of the trap remain to be investigated. In future work we plan to map out the precise phase diagram, including the location of the discontinuities, which requires extensive numerical calculations to perform the additional coupling constant integral. The presence of first-order DPTs in the FKM and the Hubbard model can shed new light on the previous works on DPTs. For example, there are indications that the nonanalyticity of the Loschmidt rate found in the Ising model [18] and its nonintegrable variants [29,32] are of first order: the analytical expressions in Ref. [18] show that the generalized expectation value of the transverse magnetization M, which is a derivative of the Loschmidt rate with respect to the magnetic field, shows a jump at the critical times. (More recent work on two-band systems indicates transitions of different order [54]). An intriguing problem would thus be to compute also conditional amplitudes (2) as a function of time and M in this exactly solvable model, and thus to characterize the analytical structure of the transition in this model.

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