Dynamics of Symmetry Breaking during Quantum Real-Time Evolution in a Minimal Model System

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One necessary criterion for the thermalization of a nonequilibrium quantum many-particle system is ergodicity. It is, however, not sufficient in cases where the asymptotic long-time state lies in a symmetry-broken phase but the initial state of nonequilibrium time evolution is fully symmetric with respect to this symmetry. In equilibrium, one particular symmetry-broken state is chosen as a result of an infinitesimal symmetry-breaking perturbation. From a dynamical point of view the question is: Can such an infinitesimal perturbation be sufficient for the system to establish a nonvanishing order during quantum real-time evolution? We study this question analytically for a minimal model system that can be associated with symmetry breaking, the ferromagnetic Kondo model. We show that after a quantum quench from a completely symmetric state the system is able to break its symmetry dynamically and discuss how these features can be observed experimentally.

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Introduction.—At the heart of thermodynamics lies the assumption that realistic macroscopic physical systems exhibit one particular state—thermal equilibrium—that is always approached irrespective of the initial condition. From a fundamental point of view the important question, however, which microscopic conditions are necessary or sufficient for the thermalization of a *closed* quantum system, is still largely unanswered [1]. This is of particular importance especially because there exists a specific class of isolated quantum systems termed integrable for which equilibration is hindered by the presence of special conservation laws, as demonstrated experimentally in the quantum version of Newton's cradle [2]. Generally, it is believed that nonintegrable systems can thermalize because they are complex enough in order to be ergodic [1].

Ergodicity, however, is not always sufficient for thermalization even though the system under study may be nonintegrable. This is the case whenever the asymptotic long-time state lies in a symmetry-broken phase, but the initial state is fully symmetric. As the Hamiltonian conserves this symmetry by construction, the system can never break this symmetry by itself, but rather requires some symmetry-breaking perturbation from the exterior. Recall that an equilibrium system in a symmetry-broken phase displays nonvanishing order as a consequence of an infinitesimal symmetry-breaking perturbation that favors one of the symmetry-broken sectors. From a theoretical point of view, this infinite sensitivity can be associated with the noncommutativity of two limits: $\lim_{h\to 0}\lim_{L\to\infty} \neq \lim_{L\to\infty}\lim_{h\to 0}$ where h refers to the strength of the symmetry-breaking perturbation (e.g., a magnetic field) and L to the system size.

In this Letter we focus on the dynamical perspective of spontaneous symmetry breaking: Consider a quantum system, with parameters placing it in a symmetry-broken phase, which is initialized in a symmetric state with vanishing order parameter. How can quantum real-time evolution break a symmetry dynamically? More specifically, can an *infinitesimal* symmetry-breaking perturbation h establish order during nonequilibrium real-time evolution? It is the aim of this work to address this fundamental question. Clearly, in a case where the order parameter M itself is a constant of motion, dynamic symmetry breaking is impossible. Here we demonstrate that, for the opposite case, symmetry breaking can indeed occur dynamically. Given that $M(t,h)$ is a continuous function of time and field with $M(t=0,h)=0$ and that $M(t,h\to 0)$ can be expected to vanish at any *finite* t, the limit $h\to 0$ has to be combined with the long-time limit $t\to\infty$. In analogy to the equilibrium case we propose the following criterion to detect the dynamical breaking of a symmetry: the noncommutativity of two limits $\lim_{h\to 0}\lim_{t\to\infty} \neq \lim_{t\to\infty}\lim_{h\to 0}$ (and system size $L\to\infty$ by default). This criterion translates the infinite sensitivity against a symmetry-breaking perturbation into the dynamical context.

In classical systems, the buildup of ordered structures out of metastable disordered states, e.g., crystallization of undercooled liquids, has been studied extensively [3]. These metastable states may either develop instabilities, such as in the context of spinodal decomposition, or decay into the respective stable thermodynamic equilibria via the formation of droplets in case of nucleation. Classical nucleation is driven by thermal fluctuations induced by a surrounding bath, but the transition from metastable to stable states may also be induced by quantum fluctuations overcoming the potential barrier between the two states via quantum tunneling [4]. Here, we will be interested in the buildup of order during unitary real-time evolution in a minimal quantum magnet far beyond equilibrium where no notion of metastable states in free-energy landscapes exists. Recently, the buildup of antiferromagnetic order in the Hubbard model has been investigated for cases where the symmetry-breaking perturbation acts over finite time intervals [5]. Moreover, for the Lieb-Mattis model it has been shown that the symmetry-breaking perturbation is not capable of inducing nonzero order except at a periodic sequence of singular points in time [6].

Ferromagnetic Kondo model.—We will demonstrate the anticipated ideas for a minimal model system, the ferromagnetic Kondo model. By a quantum-classical mapping this model is equivalent to the one-dimensional $1/r^2$-Ising chain [7], which hosts a symmetry-broken phase at low temperatures with a nonzero magnetization [8] that is triggered by an infinitesimal magnetic field. We study the dynamics of symmetry breaking for the quantum system where the symmetry breaking is associated with a boundary quantum phase transition [9] with the expectation that the main features observed are of generic relevance beyond the chosen model system. The ferromagnetic Kondo model

$$H_{\mathrm{fKM}} = \sum_{k,\sigma=\uparrow,\downarrow} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \frac{J}{2}\sum_{kk'} [c^\dagger_{k\uparrow} c_{k'\uparrow} - c^\dagger_{k\downarrow} c_{k'\downarrow}] S^z + \frac{J}{2}\sum_{kk'} [c^\dagger_{k\uparrow} c_{k'\downarrow} S^- + c^\dagger_{k\downarrow} c_{k'\uparrow} S^+] \quad (1)$$

describes a local spin-1/2 degree of freedom coupled via a ferromagnetic ($J < 0$) exchange to a fermionic bath. For the following it is suitable to introduce the dimensionless coupling constant $g = \rho J$ with ρ the noninteracting conduction band density of states that can be chosen constant within a band $[-D, D]$ for the universal properties of the model [10].

In equilibrium, the spin-1/2 becomes asymptotically free at low energies. Under a perturbative renormalization group (RG) transformation, the dimensionless coupling constant obeys the following scaling equation at low energies [10]:

$$g(\Lambda) = \frac{g}{1 + g \log(\Lambda/D)}. \quad (2)$$

The reduction of the UV-cutoff Λ well below the electronic bandwidth D leads to a logarithmic decay of g. The fixed point is thus a free theory of an isolated spin decoupled from the fermionic bath. The free spin shares a rotational symmetry that is broken by any infinitesimal local magnetic field at zero temperature forcing an alignment along the magnetic field direction. This yields a local magnetization equal to [11]

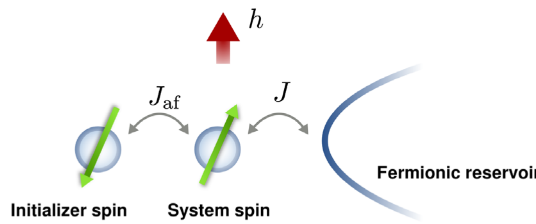

FIG. 1 (color online). Dynamics of symmetry breaking in the ferromagnetic Kondo model. The proposed setup is composed out of three elementary components. The system spin and the fermionic reservoir, coupled via a ferromagnetic exchange J, are supposed to realize the ferromagnetic Kondo model. During the dynamics of symmetry breaking in the presence of an infinitesimal local magnetic field h the system spin develops a local magnetization. The antiferromagnetic coupling J_{af} to the initializer spin generates an initially rotationally symmetric spin singlet.

$$\langle S_z \rangle = \frac{1}{2}\left[1 + \frac{g}{2} + \mathcal{O}(g^2)\right] \quad (3)$$

for a small bare coupling g. Notice that the low-energy properties of the *antiferromagnetic* Kondo model with $J > 0$ differ on a fundamental level. The system flows to strong instead of weak coupling, leading to a Kondo singlet ground state [10] which does not exhibit symmetry breaking. In order to align the local spin in this case, the magnetic field has to be sufficiently strong to overcome the binding energy of the Kondo singlet.

We develop a dynamical theory for symmetry breaking in the ferromagnetic Kondo model. Our setup is illustrated in Fig. 1. It consists of two antiferromagnetically coupled magnetic moments of spin 1/2; one of them we call the initializer spin, the other the system spin. Additionally, the system spin is also coupled to an electronic environment through a ferromagnetic exchange interaction implementing the Hamiltonian in Eq. (1). Such a ferromagnetic exchange can be realized in specific designs of triple quantum dot systems where it has been shown that it is possible to obtain effective ferromagnetic Kondo models, either anisotropic [12–14] or isotropic [15]. Notice that the initializer spin is not coupled to the electronic reservoir.

We initialize a rotationally symmetric state by decoupling the system spin from the electronic reservoir in the presence of the antiferromagnetic coupling leading to a spin singlet of the two local magnetic moments. This can be achieved by choosing J_{af} as the largest energy scale in the problem. After this initialization procedure, we switch off the antiferromagnetic coupling, inducing nonequilibrium real-time dynamics for the system spin according to the Hamiltonian in Eq. (1) while the initializer spin is decoupled from the dynamics.

We add a (infinitesimally) small magnetic field h to the system spin as the symmetry-breaking perturbation. This yields as the full Hamiltonian

$$H = H_{\rm fKM} + H_h, \qquad H_h = -hS_z. \tag{4}$$

Both the Bohr magneton and the magnetic moment's g-factor have been absorbed into the definition of the magnetic field h. In the weak-coupling limit $|g| \ll D$, our setup possesses the following hierarchy of energy scales: $|h| \lesssim |g| \ll D$. In the following we will always choose $h > 0$ for simplicity.

We study the time evolution of the local magnetization $\langle S_z(t)\rangle$ driven by the Hamiltonian H. First, we will focus on the zero-temperature limit that hosts the symmetry-broken phase of the model. Later we will also discuss the nonzero-temperature case which is of particular importance for any experimental realization. According to the anticipated protocol, the initial state $\rho_o = \rho_S \otimes \rho_B$ factorizes into the singlet $\rho_S = |S\rangle\langle S|$ of initializer and system spin and the Fermi sea ρ_B of the electronic reservoir.

Results.—We study the real-time dynamics analytically using the flow-equation technique [16] that has been proven to provide a very accurate description for the out-of-equilibrium dynamics in the ferromagnetic Kondo model. As has been shown in comparison to numerically exact time-dependent numerical renormalization group data, the flow-equation technique becomes asymptotically exact in the weak-coupling limit with well-controlled corrections for larger couplings [17].

We find that an infinitesimally small magnetic field establishes a time scale for dynamical symmetry breaking

$$t^* = \frac{\log^2(D/h)}{h} \tag{5}$$

that differs from a perturbative guess h^{-1} by a large logarithmic factor indicating its nonperturbative influence onto the system's properties. For times $t \ll t^*$, the dynamics resembles the symmetric limit with $h = 0$ up to perturbative corrections that vanish in the zero-field limit. For times $t \gg t^*$ the local moment develops a magnetization

$$\langle S_z(t)\rangle \xrightarrow{t\gg t^*} \frac{1}{2}[1+g] \tag{6}$$

whose magnitude is independent of the field strength h. The infinitesimal magnetic field h breaks the rotational symmetry and forces the system to develop a nonvanishing magnetization. Consequently, the limits $\lim_{t\to\infty}$ and $\lim_{h\to 0}$ do not commute demonstrating dynamical symmetry breaking in a quantum many-body system. Notice that the asymptotic magnetization is not thermal; compare Eq. (3) and Refs. [17–19]. It is important to note, however, that thermalization is not relevant for dynamical symmetry breaking that only relies on the noncommutativity of the limits $\lim_{t\to\infty}$ and $\lim_{h\to 0}$.

Zero temperature—The flow equation approach is an RG scheme under whose RG flow the Hamiltonian becomes more and more energy diagonal successively [16]. This is done by constructing explicitly a unitary transformation $U(B) = \mathcal{T}_B \exp[\int_0^B dB\eta(B)]$ as a B-ordered exponential of its generator $\eta(B)$ and an associated family of Hamiltonians $H(B) = U(B)HU^\dagger(B)$. For $B = 0$ one recovers the initial Hamiltonian while for $B \to \infty$ the Hamiltonian becomes diagonal in energy and exactly solvable.

For the calculation of the magnetization we introduce a novel scheme for evaluating observables within the flow equation framework that avoids the separate solution of an additional set of scaling equations for the respective observables at the same level of accuracy (see the Supplemental Material [20]). Instead, we utilize explicitly the exponential structure of the diagonalizing unitary transformation $U(B)$ by performing an operator cumulant expansion [21] as has been done in the case of the Loschmidt echo [22]. This yields for the magnetization [20]

$$\langle S_z(t)\rangle = \frac{1}{2}[e^{f_\uparrow(t)} - e^{f_\downarrow(t)}] \tag{7}$$

with $f_\sigma(t) = \int d\epsilon d\epsilon' \mathcal{J}^2_{\epsilon\epsilon'} N_{\epsilon\epsilon'}(\sigma)\{1-\cos[(\epsilon'+h^*)t]\}$, $\mathcal{J}_{\epsilon\epsilon'} = \int_0^\infty dB g^\perp_\epsilon(B)[\epsilon' + h(B)]e^{-B(\epsilon'+h(B))^2}$, and $N_{\epsilon\epsilon'}(\sigma) = n_{\epsilon-\sigma\epsilon'}(1-n_{\epsilon+\sigma\epsilon'})$ with n_ϵ the Fermi-Dirac distribution and $\sigma = \pm 1/2$ for $\sigma = \uparrow, \downarrow$. Under the RG transformation, by increasing the flow parameter B the magnetic field $h(B)$ renormalizes yielding a B dependence and asymptotically for $B \to \infty$ reaches a final value $h^* = h(B \to \infty)$. The dimensionless couplings g develop an energy dependence under the flow and the presence of a magnetic field additionally introduces an anisotropy [20,23]. For the magnetization only the renormalized spin flip coupling $g^\perp_\epsilon(B)$ enters. In Fig. 2 the results for the dynamics of the magnetization at zero temperature are shown and compared to the analytical estimates that will be presented below.

On intermediate time scales $D^{-1} \ll t \ll h^{-1}$, the two spin contributions $f_\uparrow(t) = f_\downarrow(t) = f_*$ are identical such that $\langle S^z(t)\rangle = 0$ up to perturbative corrections. Thus, the symmetry-breaking perturbation is not capable of inducing a local spin polarization in this regime. On these intermediate time scales we obtain the analytical estimate $f_* = g^2\{3 + 2\log(h/D)/[1 + g\log(h/D)]\}/2$ (see the Supplemental Material [20]) for $h > De^{1/g}$ and $f_* = g$ for $h < D^{1/g}$ which are continuously connected. In Fig. 2 we compare these analytical predictions to the numerically exact solution of the one-loop flow equations showing perfect agreement. Notice that for a fully polarized local initial state without rotational symmetry we would have $\langle S_z(t)\rangle = e^{f_*}/2 = [1 + g + \mathcal{O}(g^2)]/2$ which is precisely the result obtained in previous works [17–19], confirming the accuracy of the current calculation.

For times $t \gg t^*$, compare Eq. (5), the spin-$\uparrow$ component $f_\uparrow(t) = f_* = \text{const.}$ is frozen while the spin-$\downarrow$ component $f_\downarrow(t) = -t/t_h$ shows a linear divergence. Thus, asymptotically for large times the local spin develops a magnetization exponentially fast (see the Supplemental Material [20])

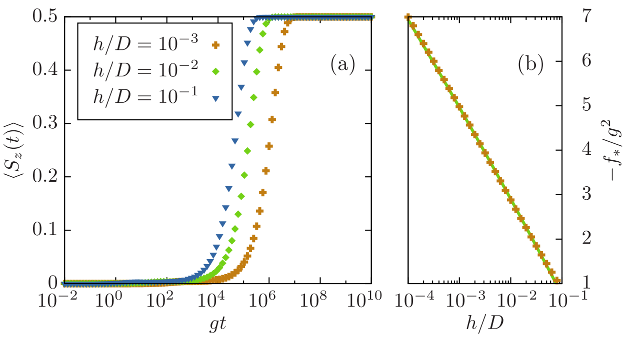

FIG. 2 (color online). (a) Dynamics of the local magnetization in the ferromagnetic Kondo model for different magnetic field strengths obtained from the numerically exact solution of the one-loop flow equations for $g = 10^{-2}$. For times $t < t^*$ the local magnetization only acquires perturbative corrections in the presence of a small magnetic field. Beyond the time scale t^*, the magnetic field induces a local magnetic moment that saturates to a value independent of the magnetic field in the asymptotic long-time limit up to corrections that vanish in the zero field limit. (b) Asymptotic long-time value of the local magnetization $\langle S_z(t\to\infty)\rangle = (1+f_*)/2$. Comparison of the full numerically exact result for f_* based on the one-loop flow equations (points) to the analytical estimate $f_*/g^2 = 3/2 + \log(h/D)/[1 + g\log(h/D)]$ (line) demonstrating the accuracy of both the numerical as well as the analytical result.

$$\langle S^z(t)\rangle \xrightarrow{t\gg t^*} \frac{1}{2}[1+f_*] - \frac{1}{2}[1+f_*]e^{-t/t_h}, \tag{8}$$

with a relaxation time

$$t_h = \sqrt{\frac{8}{\pi}}\left[\frac{1+g\log(h/D)}{g}\right]^2 \frac{1}{h}. \tag{9}$$

In the zero-field limit, one obtains to leading order $t_h \to \sqrt{8/\pi}t_*$ yielding the desired result in Eq. (5). Notice the relation to the linear-response spin relaxation rate $\Gamma \propto t_*^{-1}$ [24].

Nonzero temperatures.—In equilibrium, the local magnetization in the ferromagnetic Kondo model is nonvanishing only at zero temperature. This poses a severe challenge onto the possibility to observe the anticipated dynamical symmetry breaking in experiments that necessarily operate at nonzero temperatures. We will demonstrate below that although any nonzero temperature will eventually lead to a completely symmetric state with vanishing magnetization, this will happen only beyond a time scale t_T. On intermediate times $t < t_T$ it is possible to observe dynamical symmetry breaking provided temperature is sufficiently small such that $t_T \gtrsim t_h$; see Eq. (9). Notice that temperature also influences the preparation of the initial local singlet such that it is necessary to ensure that $J_{\mathrm{af}} \gg T$.

While to leading order any nonzero temperature will not influence the properties of $f_\downarrow(t)$, its influence onto the spin-$\uparrow$ component $f_\uparrow(t)$ is substantial for times $t \gg t_T$ with

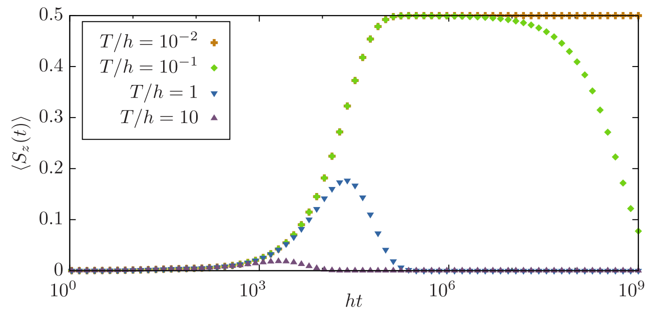

FIG. 3 (color online). Influence of temperature onto dynamical symmetry breaking in the ferromagnetic Kondo model. Dynamics of the local magnetization for different temperatures with $g = 10^{-2}$ and $h/D = 10^{-4}$. For small times $t < t_T$, see Eq. (10); the real-time evolution of the magnetization is equivalent to the zero-temperature limit demonstrating the observability of dynamical symmetry breaking in the ferromagnetic Kondo model at nonzero temperatures. Increasing temperature such that $t_T \lesssim t_*$ destroys the signatures of symmetry breaking eventually leading to a complete suppression in the limit $T \gg h$.

$$t_T = \left[\frac{1+g\log(h/D)}{g}\right]^2 \frac{e^{h/T}-1}{\pi h}, \tag{10}$$

where $f_\uparrow(t) = -t/t_T$ such that temperature induces an exponential decay of the magnetization

$$\langle S_z(t)\rangle \xrightarrow{t\gg t_T} \frac{1}{2}[1+f_*]e^{-t/t_T}, \tag{11}$$

reestablishing a completely symmetric state. For $h \gg T$ we have that $t_T \sim e^{h/T}$ yielding a symmetry-broken magnetization plateau which becomes stabilized to exponentially long times. This changes as soon as $h \lesssim T$ where $t_T \sim T^{-1}$ and $t_T \lesssim t_h$ preventing the buildup of a substantial magnetization plateau. In Fig. (3), the real-time evolution of the magnetization and its dependence on temperature is shown, confirming the analytical arguments.

Conclusion.—We have discussed the possibility of symmetry breaking induced by unitary quantum real-time evolution and its implication for fundamental concepts such as quantum ergodicity. For a minimal quantum magnet, described by the ferromagnetic Kondo model, we have demonstrated that symmetries can be broken dynamically. Based on the analytical solution of the quantum real-time evolution we showed that the system develops a nonzero local magnetization even in the limit where the symmetry-breaking magnetic field h is infinitesimally small. This implies the noncommutativity of the two limits $h \to 0$ and time $t \to \infty$ which we have identified as a general dynamical criterion for symmetry breaking.

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