Arrested states formed on quenching spin chains with competing interactions and conserved dynamics

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We study the effects of rapidly cooling to $T=0$ a spin chain with conserved dynamics and competing interactions. Depending on the degree of competition, the system is found to get arrested in different kinds of metastable states. The most interesting of these has an inhomogeneous mixture of interspersed active and quiescent regions. In this state, the steady-state autocorrelation function decays as a stretched exponential $\sim\exp[-(t/\tau_0)^{1/3}]$, and there is a two-step relaxation to equilibrium when the temperature is raised slightly. [S1063-651X(99)03009-3]

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When a system at a high temperature is cooled rapidly to low temperatures, it may not be able to reach an equilibrium state in an experimentally realizable time. Instead it may reach a long-lived arrested state, often with a degree of spatial disorder, which ultimately relaxes towards equilibrium over very much longer time scales. An intriguing possibility is that the disorder induced by the kinetics may be strong enough that the system has widely different levels of dynamical activity in distinct regions of space. Dynamically heterogeneous states are found to arise, for instance, in a glass-forming liquid [1]. From the theoretical point of view it is important to ask: Are there simple models in which dynamically heterogeneous states arise naturally? Can their formation and properties be understood in microscopic terms? Finally, how do such states decay, and how is equilibrium approached?

We address these questions by studying nonequilibrium quenches to $T=0$, in simple lattice models. Following such quenches, the system may get arrested in a metastable state instead of reaching the ground state. A useful way to characterize the resulting arrested state is to ask whether or not there is any dynamical activity in it. A *quiescent* arrested state is one in which the system settles into a single configuration, and degrees of freedom are frozen. Another possibility is that the arrested state may involve a large number of configurations which are dynamically accessible from each other; in that case the system is dynamically *active*. Interestingly, all these possibilities are realized in quenches of a family of simple models, namely, Ising chains with different degrees of competition and conservation laws. In the absence of competition, the system approaches the ground state if the dynamics is nonconserving [2], while it reaches a quiescent arrested state under spin-conserving dynamics [3]. On the other hand, a system with competing interactions, evolving under nonconserved dynamics, has been shown to exhibit an active arrested state [4]. This naturally leads to the question: Are new features brought in if both conservation and competition are present? In this paper, we study the effects of quenching the simplest model which incorporates both these features, namely, an Ising model with competing first and second neighbor interactions, evolving through a dynamics with a single conservation law. Despite its simplicity, the model shows interesting transitions in the character of the arrested states as the degree of competition is varied (Fig. 1). The most interesting of these arrested states, reached for strong enough competition, is of a qualitatively new type: it has active and quiescent regions interspersed in a disordered fashion throughout the system. This *inhomogeneous quiescent and active* (IQA) state has nontrivial dynamical properties. In the $T=0$ steady state the autocorrelation function has a stretched exponential decay. Further, if the temperature is raised slightly, there is a two-step relaxation: the IQA state relaxes to equilibrium via an intermediate long-lived intermediate energy state. We are able to quantitatively understand many of these unusual features, often found in glassy systems, within this simple model.

The equilibrium phases and transitions of the axial next-nearest-neighbor Ising (ANNNI) model have been well studied and characterized [5]. However, its nonequilibrium properties remain relatively unexplored even in one dimension (1D), except for a few studies. An early such study explored arrested states obtained by quenching across $T=0$ phase boundaries of an extended ANNNI model appropriate to polytypes [6]. More recently, time-dependent coarsening induced by nonconserved dynamics has also been studied by quenching the system across phase boundaries at $T=0$ [7], and also from $T=\infty$ to $T=0$ [4]. Here we explore the interplay of competing interactions with conservation laws in the dynamics. Our principal result is the identification and char-

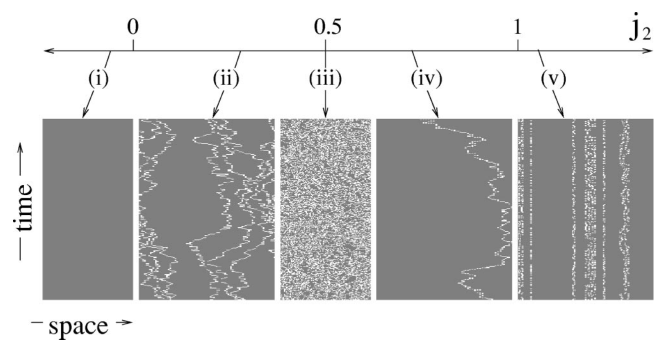

FIG. 1. Space-time depiction of the activity (shown white) in different arrested states. Different regimes: (i) Quiescent, (ii) mobile domain walls, (iii) active, (iv) essentially quiescent, and (v) IQA state.

acterization of an IQA arrested state in this system.

Consider an Ising chain with spin variables $\{s_i\}$ described by the Hamiltonian

$$\mathcal{H}=-J_1\sum_i s_i s_{i+1}+J_2\sum_i s_i s_{i+2}. \tag{1}$$

An antiferromagnetic next-neighbor coupling ($J_2>0$) competes with the nearest-neighbor coupling J_1 which may be of either sign. In what follows, we shall assume $J_1>0$ (ferromagnetic coupling) and define $j_2=J_2/J_1$ as a measure of the strength of competition. The equilibrium ground state shows a transition from the ferromagnetic state $\uparrow\uparrow\uparrow\uparrow\ldots$ for $j_2<0.5$, to the antiphase state $\uparrow\uparrow\downarrow\downarrow\ldots$ for $j_2>0.5$. The point $j_2=0.5$ is a multiphase point, at which the number of ground states (all configurations with no single spins) is exponentially large in system size L [5]. We are interested in the effect of a quench from an infinite-temperature random configuration of the system to $T=0$. We use a double-spin-flip dynamics (DSFD), in which an adjacent pair of randomly chosen parallel spins is flipped ($\ldots\uparrow\uparrow\ldots\rightarrow\ldots\downarrow\downarrow\ldots$). Flips are attempted at unit rate, and are allowed only if the energy is not raised ($\Delta E\leqslant 0$). Evidently, the DSFD conserves the difference $M=M_1-M_2$ of the two sublattice magnetizations M_1 and M_2. The dynamics thus involves a single conservation law. The DSFD maps onto the well-known Kawasaki spin exchange dynamics through a sublattice mapping, in which every spin on one of the two sublattices is inverted and the sign of the nearest-neighbor coupling J_1 is reversed. In the mapped model with Kawasaki dynamics, M is the total conserved magnetization. We will use the DSFD, rather than Kawasaki description; results can be translated readily. The DSFD can be looked upon as an extension of the single-spin-flip Glauber dynamics to multiple-spin flips at a time. Multispin moves arise in physical contexts such as stacking dynamics in the $3C$-$6H$ transition in SiC [8] and deposition-evaporation dynamics of bunches of particles [9].

The energy nonraising condition, which is a consequence of a $T=0$ quench, imposes local constraints on whether or not a pair of chosen spins can actually be flipped; these constraints are a function of j_2. The normalized energy changes $\Delta e\equiv\Delta E/J_1$ involved in flipping a pair $\uparrow\uparrow$ to $\downarrow\downarrow$ depend on the environments of the pair, and are given in Eq. 2 below. There are six distinct local environments; the other unlisted environments are related to these by reflection symmetries.

$$\begin{array}{llcll}
(a) & \Uparrow\Downarrow\uparrow\uparrow\Downarrow\Downarrow & \rightarrow & \Uparrow\Downarrow\downarrow\downarrow\Downarrow\Downarrow & \Delta e=-(4-4j_2),\\
(b) & \Downarrow\Uparrow\uparrow\uparrow\Uparrow\Downarrow & \rightarrow & \Downarrow\Uparrow\downarrow\downarrow\Uparrow\Downarrow & \Delta e=4,\\
(c) & \Downarrow\Uparrow\uparrow\uparrow\Downarrow\Downarrow & \rightarrow & \Downarrow\Uparrow\downarrow\downarrow\Downarrow\Downarrow & \Delta e=4j_2,\\
(d) & \Downarrow\Downarrow\uparrow\uparrow\Downarrow\Downarrow & \rightarrow & \Downarrow\Downarrow\downarrow\downarrow\Downarrow\Downarrow & \Delta e=-(4-8j_2),\\
(e) & \Downarrow\Uparrow\uparrow\uparrow\Downarrow\Uparrow & \rightarrow & \Downarrow\Uparrow\downarrow\downarrow\Downarrow\Uparrow & \Delta e=0,\\
(f) & \Downarrow\Downarrow\uparrow\uparrow\Uparrow\Uparrow & \rightarrow & \Downarrow\Downarrow\downarrow\downarrow\Uparrow\Uparrow & \Delta e=0.
\end{array} \tag{2}$$

The reverse of move (a) in Eq. (2) will be referred to as $(\bar{a})$, and similarly for the others.

Evidently the dynamics is identical for all values of j_2 for which the same set of moves are allowed. Moves $(\bar{b})$, (e), $(\bar{e})$, (f), and $(\bar{f})$ are allowed (i.e., $\Delta e\leqslant 0$) for all j_2. As j_2 is varied, Δe changes sign for moves (a), (c), and (d). Each such change causes a change in the nature of the arrested state. While (c) is an allowed move for $j_2<0$, $(\bar{c})$ becomes an allowed move for $j_2>0$. Similarly, across $j_2=0.5$ and $j_2=1$, the allowed moves change from (d) to $(\bar{d})$ and (a) to $(\bar{a})$, respectively. Thus there are distinct regions of dynamical activity along the j_2 axis: (i) $j_2\in(-\infty,0)$, (ii) $j_2\in[0,0.5)$, (iii) $j_2=0.5$, (iv) $j_2\in(0.5,1]$, and (v) $j_2\in(1,\infty)$; see Fig. 1. In region (v), i.e., for strong competition, the system reaches an IQA arrested state.

We used Monte Carlo simulation to study the arrested steady states that are reached under $\Delta e\leqslant 0$ DSFD starting from a random initial configuration corresponding to $T=\infty$. We studied the approach to the arrested states, the dynamical behavior in these states, and finally the relaxation from these states to equilibrium at low but finite temperatures. The approach to, and the decay from, the steady state was monitored by following the decay of the energy in time. Further, in cases (iii) and (v), we studied the dynamical behavior of the steady state by monitoring the spin-spin autocorrelation function

$$C(t)=\frac{1}{N}\sum_i \langle s_i(t_0)s_i(t_0+t)\rangle-\langle s_i(t_0)\rangle^2, \tag{3}$$

where t is the number of Monte Carlo steps per spin and $\langle\ldots\rangle$ denotes an average over t_0. We allowed for an explicit dependence of averages on the space location i, as arrested states need not be translationally invariant. Only at the multiphase point (iii) is the ground state reached on quenching; in the other four regions of j_2 discussed above (Fig. 1), the steady states are arrested.

Before discussing the IQA state in detail, we sketch some features of the states in the other four regions.

(i) The arrested state is quiescent. It consists of ferromagnetic patches separated by clusters of frozen domain walls, e.g., $\ldots\uparrow\uparrow\uparrow\uparrow\downarrow\uparrow\downarrow\uparrow\uparrow\uparrow\ldots$. It is qualitatively similar to the arrested state obtained in [3], with only first-neighbor interactions.

(ii) The steady state has a number of diffusing domain walls separating ferromagnetically aligned patches (Fig. 1). Though it resembles the active arrested states found in [4], there is an important difference. The level of activity is much lower in our case, as the number of walls increases as $\sim L^{1/2}$ as opposed to $\sim L$ in [4].

(iii) At the multiphase point there is a large degree of activity (Fig. 1), because the $\Delta e=0$ moves (d), (f) and their reverses carry the system through a subspace of ground-state configurations labeled by a given value of M. The autocorrelation function $C(t)\sim t^{-1/2}$ at long times, as in the unconstrained DFSD [9].

(iv) The steady state has alternating opposite-spin clusters of two or three spins, e.g., $\ldots\downarrow\downarrow\downarrow\uparrow\uparrow\downarrow\downarrow\downarrow\uparrow\uparrow\uparrow\ldots$, and is quiescent. A single cluster of four or five spins may remain in the steady state and diffuse through a quiescent background (Fig. 1).

In region (v), an IQA arrested state with alternating quiescent and active stretches is reached. A segment of a typical configuration is depicted below.

..[⇓⇑⇑⇓⇓⇑] ↓↑↓↓↓↑↓↑↓↑↑↑↓↑↓ [⇑⇓⇓⇑⇑⇑⇓⇓⇑⇓⇓⇑⇑⇑⇓⇓⇑]..

Quiescent Active Quiescent

Each active region has parallel-spin triplets in a background of alternating single spins, while the quiescent portions predominantly resemble the arrested state of region (iv). Crucial to the coexistence of active and quiescent regions is the existence of stable walls at the boundaries of quiescent regions. These consist of left boundaries ⇑⇓⇓ or ⇓⇑⇑ and right boundaries ⇓⇓⇑ or ⇑⇑⇓, and are stable as moves (a) and (c) are energy raising for $j_2 > 1$. The numbers of quiescent and active (q and a, respectively) regions of size $\tilde{l}$ are found numerically to decay as $\exp(-\lambda\tilde{l})$ with $\lambda_q \simeq 0.05$ and $\lambda_a \simeq 0.25$.

We now turn to the dynamical properties of the IQA state. The *autocorrelation function* in the steady state decays as a stretched exponential $\sim\exp(-(t/\tau_0)^{1/3})$ (Fig. 2). Interestingly, the dynamical behavior of the IQA state can be related to the well-known symmetric exclusion process (SEP) of particles on a line [10]. This can be understood as follows. Each spin triplet in an active stretch can move by one unit right or left, under the DSFD move (e) $(\ldots\downarrow\uparrow\downarrow\overline{\uparrow\uparrow\uparrow}\downarrow\uparrow\ldots\leftrightarrow\ldots\downarrow\uparrow\overline{\downarrow\downarrow\downarrow}\uparrow\downarrow\uparrow\ldots)$. There is a hard-core repulsion between triplets as move (c) is disallowed. The dynamics within a single active region is thus precisely that of a symmetric exclusion process of hard triplets on a lattice, where the single spins can be viewed as holes. The autocorrelation function $C_{\tilde{l}}(\rho,t)$ averaged over spins, of an active stretch of length $\tilde{l}$ with ρl triplets (where $l=\tilde{l}+2$ and $1/l \leqslant \rho \leqslant 1/3$), is thus governed by the diffusion of these hard triplets; triplets extend over an extra lattice unit at both boundaries of an active stretch, making its effective length l. Hence, we expect $C_{\tilde{l}}(\rho,t)$ to decay as $t^{-1/2}$ for times t less than a cutoff time $\tau_l(\rho)$, and as $\exp(-t/\tau_l(\rho))$ thereafter. Further, $\tau_l(\rho)$ can be found by noting an exact mapping of every configuration of this problem to a corresponding configuration of the SEP. Under the mapping, every triplet is replaced by a single particle, while a single spin maps onto a hole (↑↓↑↓↓↓↑↓↑↑↑↓↓↓↑↓ →○○○●○○●●○○). The mapped chain has a reduced length $l' = l(1-2\rho)$. The stochastic $\mathcal{W}$ matrices for the two processes are the same, as there is a one-to-one correspondence between configurations and moves. This implies that the eigenvalue spectra of the $\mathcal{W}$ matrices in the two problems are the same, and in particular, the gap Δ_l to the first excited state is the same. The inverse of the gap is just the cutoff time τ_l, and so the above equality implies $\tau_l = \tau'_{l'}$. For the exclusion process, with free boundary conditions $\tau'_{l'} = 2l'^2/\pi^2$ for large l' (the diffusion constant equals $\frac{1}{2}$) [11], and hence $\tau_l(\rho) = 2l^2(1-2\rho)^2/\pi^2$.

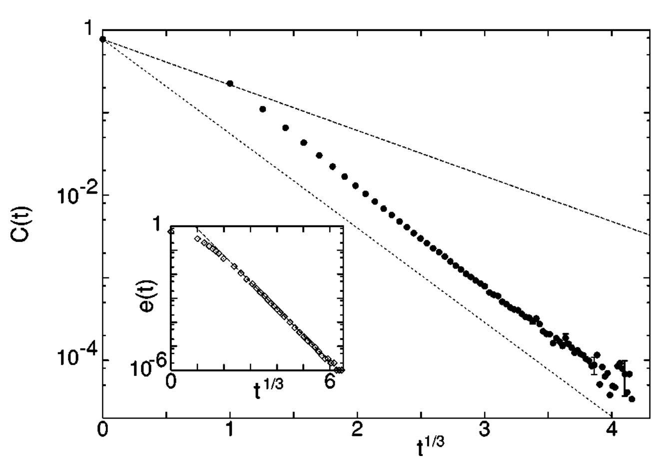

FIG. 2. The autocorrelation function in the IQA state with $L = 12\,000$ and 10^6 histories. The dotted curves are the bounds discussed in the text. Inset: Decay of energy excess (in units of J_1) over the IQA value, starting from a random state.

The autocorrelation function $C_{\mathrm{IQA}}(t)$ of the IQA state can be expressed in terms of a sum over active stretches:

$$C_{\mathrm{IQA}}(t) = \sum_{\tilde{l},\rho} P_{\tilde{l}}(\rho) C_{\tilde{l}}(\rho,t), \tag{4}$$

where $P_{\tilde{l}}(\rho)$ is the probability of finding an active stretch of length $\tilde{l}$ and density ρ of triplets. Even without explicitly determining $P_{\tilde{l}}(\rho)$, we can derive bounds on $C_{\mathrm{IQA}}(t)$ using $P_{\tilde{l}} = \Sigma_\rho P_{\tilde{l}}(\rho) \sim \exp(-\lambda_a \tilde{l})$. As ρ varies across its range, the cutoff time τ_l varies between the two limits $\tau_l(0) = 2l^2/\pi^2$ (for a single triplet) and $\tau_l(\frac{1}{3}) = 2l^2/9\pi^2$ (for a single hole hopping over three lattice units at a time). For each of these limits $\tau_l(\rho^*)$, the sum in Eq. (4) is dominated at long times by the term with the saddle point value $l^* = [t\pi^2/\lambda_a(1-2\rho^*)^2]^{1/3}$. The bounds imply that C_{IQA} has a stretched exponential form $\sim\exp[-(t/\tau_0)^{1/3}]$, with $8/243\pi^2 \leqslant \tau_0\lambda_a^2 \leqslant 8/27\pi^2$. The numerically determined values $\tau_0 \simeq 0.08$ and $\lambda_a \simeq 0.25$ are consistent with these bounds (Fig. 2).

The *dynamics of approach* to the IQA state, starting from a random initial configuration, is also interesting. From numerical simulations the energy is found to decay as $\sim\exp[-(t/t_0)^{1/3}]$ (see inset in Fig. 2). This is associated primarily with the fall in the number N_4 of four-spin clusters which diffuse through ground-state stretches $\ldots\uparrow\uparrow\downarrow\downarrow\ldots$ until they dissociate when they encounter ''traps'' in the form of a single spin or a triplet; e.g., $\ldots\uparrow\uparrow\downarrow\uparrow\uparrow\uparrow\ldots \rightarrow \ldots\uparrow\uparrow\downarrow\downarrow\downarrow\uparrow\uparrow\ldots$. The typical time for a four cluster to diffuse over a length l before encountering such a trap is l^2/D, implying that $N_4(l)$ decays as $\exp(-Dt/l^2)$. Further, the stretch lengths are distributed exponentially $\sim\exp(-\lambda l)$, so that the average of $N_4(l)$ over l is dominated by a saddle point value $l^* = (2Dt/\lambda)^{1/3}$ at large t. This argument is reminiscent of that in [12] and implies a stretched exponential form for the decay.

Finally, let us discuss the *relaxation to equilibrium* from the IQA arrested state. The IQA state has regions with two distinct types of excitations, namely, active patches with

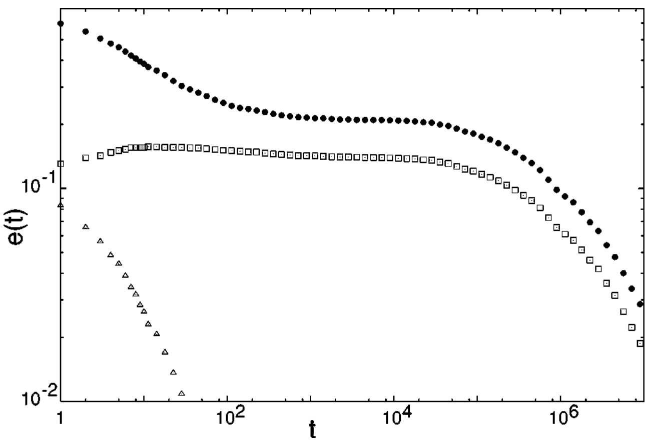

FIG. 3. Energy per site $e(t)$ (●) in units of J_1, measured from the ground-state value, when the IQA state is taken to $T \simeq 0.29 J_1$. We used $\omega_a = 1$, $\omega_c = 0.9 \times 10^{-6}$, $L = 1200$, and 12 initial conditions. Also shown are the fraction of single spins (△) and triplets (□).

mostly single spins (and occasional mobile triplets) and quiescent patches with mostly triplets (and occasional frozen single spins). If T is raised to a small value, the system relaxes to an equilibrium state close to the $\ldots\uparrow\uparrow\downarrow\downarrow\ldots$ ground state, by annealing out both the single-spin and triplet excitations. Figure 3 shows the subsequent variation of energy with time. There is a relatively rapid approach to a second metastable state, evidenced by a long plateau (Fig. 3), followed by an eventual approach to equilibrium. This can be understood as follows. For finite T, the energy raising moves (a), (b), (c), and (d) are allowed, with probabilities $\omega_k \sim \exp(-\Delta e_k/T)$, $k = a,b,c,d$; the associated time scales are $\sim 1/\omega_k$. Moves (a) and (c) are instrumental in annealing out the two different kinds of local excitations (isolated spins and triplets, respectively). They act on time scales which are widely different $[\omega_c^{-1}/\omega_a^{-1} \sim \exp(4J_1/T)]$ leading to the plateau. For small t, i.e., $t \sim \omega_a^{-1}$, only move (a) is effective, which destabilizes active-quiescent boundaries and creates five-spin clusters. Single spins diffuse out of active stretches and annihilate on meeting five clusters, e.g., $\downarrow\downarrow\uparrow\downarrow\downarrow\downarrow\downarrow \rightarrow \downarrow\downarrow\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow$. After the single spins anneal out, the system reaches a metastable state with clusters of length 2 and 3, much like the arrested state in region (iv). This continues till $t \gtrsim \omega_c^{-1}$, when triplets begin to decay. To leading order in low T, the predominant decay channel involves the following steps: (i) the conversion of a triplet to a single spin and a four-spin cluster (at rate ω_c), (ii) the production of a single spin when the four cluster meets the nearest triplet, and (iii) the fast diffusion of single spins till they meet triplets or single spins at separation $2n$ (n = odd), whereupon they annihilate, e.g., $\downarrow\downarrow\uparrow\downarrow\downarrow\uparrow\uparrow\uparrow \rightarrow \downarrow\downarrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow \rightarrow \downarrow\downarrow\uparrow\uparrow\downarrow\downarrow\uparrow\uparrow$. Process (iii) is a variant of the single species diffusion-annihilation process [13], implying a power-law ($\sim t^{-1/2}$) decay for the energy.

To summarize, a simple understanding of the dynamics of the IQA state can be achieved in terms of diffusing excitations; the nature of approach, steady-state autocorrelation function, and decay of the state involve variants of the diffusion problem. For instance, the approach to the IQA state involves diffusion in the presence of randomly placed traps, while the autocorrelation function involves the consequences of confinement of diffusing excitations in active stretches of random lengths. In both cases, an average over the dynamically generated randomness results in a stretched exponential decay. The two distinct time scales for relaxation from the IQA state arise from the different activation rates for the two types of diffusing excitations. Diffusion-limited annihilation of the second type governs the power-law decay towards equilibrium.

We conclude by pointing out that IQA arrested states occur in several other situations, for instance, with antiferromagnetic nearest-neighbor coupling ($J_1 < 0$), and also under a quench to region (v) from a quiescent arrested state in region (i). Further, an IQA state is found in quenches of an extended ANNNI model relevant to polytype transitions. This model is richer, and shows variability in the microscopic nature of activity in IQA arrested states for different parameter values [14]. Interestingly, despite this variation, the dynamical behavior remains of the same form—a general consequence of the diffusion-based description given above.

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