Irreversible phase transitions induced by an oscillatory input

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Abstract. – A novel kind of irreversible phase transitions (IPTs) driven by an oscillatory input parameter is studied by means of computer simulations. Second-order IPTs showing scale invariance in relevant dynamic critical properties are found to belong to the universality class of directed percolation. In contrast, the absence of scale invariance is observed for first-order IPTs.

Far from equilibrium systems often exhibit irreversible phase transitions (IPTs) between an active (or reactive) regime and an inactive (or absorbing) state. Such transitions are irreversible because a system trapped in an absorbing state can never escape from it. Among others, models exhibiting IPTs are directed percolation [1], contact processes [2], branching annihilating walkers [3], forest fire models [4–6], models of the dynamic evolution of living individuals [7] and several models of catalyzed reactions such as the Ziff-Gulari-Barshad (ZGB) model [8] and its variations [9,10].

In spite of the considerable progress achieved in the understanding of irreversible critical behavior (for reviews see, e.g., [9–11]), the study of the dynamic response of irreversible systems to external perturbations is still in its infancy. Very recently, we have studied the dynamic response of the ZGB model close to a second-order IPT, showing that the relaxation of the system after it is suddenly stepped across the IPT into the absorbing state, can be well described by a stretched exponential decay [12]. The lack of additional studies in the field of non-equilibrium phase transitions is in contrast with its equilibrium counterpart. In fact, the study of the dynamic response of systems in thermodynamic equilibrium, close to reversible phase transitions, to an external perturbation, is a subject of current interest [13].

The aim of this work is to study the dynamic response of irreversible systems to a periodic external perturbation. The study has been performed close to both first- and second-order

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IPTs. For this purpose we have selected a forest fire model with immune trees (FFMIT) [5] and the ZGB model [8].

The ZGB model is a lattice gas reaction system aimed to mimic the catalytic oxidation of carbon monoxide, \( \text{CO} + (1/2)\text{O}_2 \rightarrow \text{CO}_2 \), according to the Langmuir-Hinshelwood mechanism. So, \( \text{CO} \) and \( \text{O}_2 \) molecules in the gas phase may become adsorbed on the surface of the catalyst with probabilities \( P_{\text{CO}} \) and \( P_{\text{O}_2} \), respectively. Since these probabilities are normalized \( (P_{\text{CO}} + P_{\text{O}_2} = 1) \), the ZGB model has a single parameter, \( i.e. P_{\text{CO}} \). For \( P_{\text{CO}} \rightarrow 1 (P_{\text{CO}} \rightarrow 0) \), the surface of the catalyst becomes inactive due to complete saturation with \( \text{CO} (\text{O}) \) species, respectively. Monte Carlo simulations performed in the square lattice show that between these two inactive states there is a reactive regime as is shown in fig. 1. Close to \( P_{2\text{CO}} \simeq 0.5256 \) the ZGB exhibits an abrupt change in the rate of reaction and reactant's coverages, as is shown in fig. 1, indicating a first-order IPT. Further details on the ZGB model can be found elsewhere [9].

In order to study the dynamic response of this system close to the first-order IPT, first a stationary configuration of the ZGB model well inside the reactive regime (actually in the center of the reaction window \( P_{\text{CO}}^w = 0.455 \)) is obtained. Subsequently, a periodic-square oscillatory perturbation of the form

\[
P_{\text{CO}}(t) = \begin{cases} 
P_{\text{CO}}^w + A_{\text{PCO}}, & \text{if } 0 \leq t < \tau/2, \\
P_{\text{CO}}^w, & \text{if } \tau/2 \leq t < \tau, \\
P_{\text{CO}}(t + \tau), & \forall t \geq 0 
\end{cases}
\]

(1)

is applied to the system, where \( A_{\text{PCO}} \) is the amplitude and \( \tau \) is the period of the perturbation (see also fig. 1).

On the other hand, to study the dynamic response of a system close to a second-order IPT, we have selected a forest fire model (FFM), \( e.g. [4-6] \). FFM are stochastic cellular automata which are defined on \( d \)-dimensional hypercube lattices with \( L^d \) sites. Each site can be either occupied by a tree, a burning tree, or empty. These FFM can be defined giving a set of rules which are used, during each time step, to update the system in parallel. These rules are: 1) burning tree \( \rightarrow \) empty site; 2) tree \( \rightarrow \) burning tree with probability \( (1 - g) \) if at least one
nearest neighbor is burning; and 3) empty site → tree with probability $p$. The probability $p$ is taken to be the growing probability and $g$ is the immunity of each tree to catch fire.

In the present work we shall focus our attention to the forest fire model with immune trees (FFMIT), without lightnings [4–6]. Qualitatively speaking, if the growing probability is large (but $p < 1$) and the immunity is low (but $g > 0$) one expects coexistence of fire, trees and empty sites. However, keeping $p$ constant and increasing $g$ the fire will eventually cease and the system will become irreversibly trapped in an absorbing state with the lattice completely filled by trees. So, the FFMIT exhibits second-order IPTs between active states with fire propagation and a single absorbing state where the fire becomes irreversibly extinguished [4,6].

In order to study the dynamic response of the FFMIT upon temporal variations of the parameters, one can vary either $p$, $g$, or both of them. However, we have worked taking $p =$ const while $g$ is varied. For this purpose, the procedure is as follows: first a stationary active state of the standard FFMIT is obtained for fixed values of the parameters. In this work we take $p = p_0 = 0.5$ and $g = g_0 = 0.46$. Subsequently, $p$ is kept fixed and $g$ is varied harmonically according to

$$g = \left( g_0 + \frac{A_g}{2} \right) + \frac{A_g}{2} \sin \left( \frac{2\pi}{T} t \right),$$

where $A_g$ and $T$ are the amplitude and the period of the oscillation, respectively. Notice that the critical point is given by $p_0 = p_c = 0.5$ and $g_c = 0.5614 \pm 0.0005$ [4,6].

Due to the variation of the parameters, either $g(t)$ or $P_{CO}(t)$, it is expected that for long periods and/or large amplitudes, the systems may eventually become trapped into the absorbing state. So, the oscillatory variation of the parameters may cause IPTs from the active (oscillatory) regimes to the absorbing state. These transitions may occur at critical values of the amplitude ($A_g^c$ and $A_{P_{CO}}^c$) and the period ($T_c$ and $\tau_c$). In order to characterize and study such IPTs, we have performed epidemic simulations (ES) [1–4]. The idea behind ES is to start from a configuration very close to the absorbing state and subsequently, to follow the temporal evolution of the system under consideration. Therefore, we take a sample filled with trees except for a small patch of $2 \times 2$ sites having burning trees placed at the center of the lattice for the FFMIT. For the ZGB model, the sample has to be filled by CO-molecules, while the sites of the small patch are left empty. During the epidemic propagation the following quantities are measured: i) the average number of burning trees (empty sites) $N(t)$, respectively; ii) the survival probability $P(t)$, i.e. the probability that the fire is still ignited (there are empty sites) at time $t$, respectively; and iii) the average mean-square distance $R^2(t)$ over which the fire (empty sites) has spread, respectively.

Figure 2(a) shows a log-log plot of $N(t)$ vs. $t$ obtained by performing ES of the FFMIT, where the influence of the oscillatory input can clearly be observed. The inset of the right-hand side of fig. 2(a) shows the results of a Fourier analysis of the time series $N(t)$ at criticality. It is observed that the input period dominates the spectrum, the first harmonic has a rather small amplitude, while the second harmonic is vanishingly small. No evidence of relevant anharmonic terms are found.

The usual ansatz for ES close to second-order IPTs is to assume that $N(t)$, $P(t)$ and $R^2(t)$ would obey power law dependencies with exponents $\eta$, $-\delta$ and $z$ [1], respectively. However, in the present ES of the FFMIT the input parameter varies harmonically, so we expect to obtain an oscillatory output modulated by a power law, that is

$$N(t) = N_0 + t^\eta \left( N_1 + N_2 \cos \left( \frac{2\pi}{T} t + B \right) \right),$$

where $A_g$ and $T$ are the amplitude and the period of the oscillation, respectively. Notice that the critical point is given by $p_0 = p_c = 0.5$ and $g_c = 0.5614 \pm 0.0005$ [4,6].

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Fig. 2 – Results for the FFMIT obtained by performing ES. (a) Log-log plot of $N(t)$ vs. $t$ with $A_g = 0.1695$ and $T = 55$. The upper left inset shows log-log plots of $N^+, N^-$ and $N^0$ vs. $t$ (see text). The upper right inset shows the results of a Fourier analysis through an amplitude spectrum of the time series of $N(t)$ at criticality. The location of the first harmonics are shown by arrows (more details in the text). (b) Fit of $N(t)$ vs. $t$ (see text). The inset shows the constant phase shift $B$ between input and the output signal.

where $N_0$ is the initial number of burning trees, $N_1$ and $N_2$ are equation constants. $B$ is a constant phase shift. Similar ansätze can be proposed for $P(t)$ and $R^2(t)$. Notice that anharmonic contributions are not considered in eq. (3) in view of the results of the Fourier analysis, as discussed above.

In order to perform a fit, we have first determined the values of $N(t)$ on peaks, valleys and centers, given by $N^+, N^-$ and $N^0$, respectively. The inset of fig. 2(a) shows that log-log plots of $N^+, N^-$ and $N^0$ vs. $t$ can be very well fitted by straight lines with slopes $\eta^+ = 0.22 \pm 0.02$, $\eta^- = 0.22 \pm 0.02$, and $\eta^0 = 0.22 \pm 0.02$, respectively. Notice that error bars only account for the statistical errors. As is usual, plots drawn taking smaller (larger) amplitudes show upward (downward) curvature suggesting that they are off-criticality, respectively. Precisely, the straight line observed is the signature of a power law behavior which characterizes a second-order phase transition exhibiting scale invariance. The inset in fig. 2(b) shows that it is also possible to determine the assumed constant phase shift in eq. (3), comparing plots of $N(t)$ and $g(t)$ vs. $t$. For example, in fig. 2(b), we have obtained $B = 1.37 \pm 0.34$. It should be notice that $B$ remains constant, within error bars, for the whole time series of $N(t)$ vs. $t$ in agreement with the lack of evidences of anharmonic terms found using the Fourier analysis (fig. 2(a)). Therefore we can fit the whole curve of $N(t)$ vs. $t$ in each cycle as $P^+$, $P^-$ and $P^0$, respectively, we can fit the

Figure 3 shows a log-log plot of $P(t)$ vs. $t$ which also exhibits oscillatory behavior. In this case, the drops of the survival probability are due to the increment in the immunity which drives the system into the absorbing state making the fire propagation harder, an effect which may cause the eventual extinction of some epidemics. Defining the maximum, medium and minimum values of $P(t)$ in each cycle as $P^+, P^-$ and $P^0$, respectively, we can fit the
Fig. 3 – Log-log plot of $P(t)$ vs. $t$ obtained by performing ES for the FFMIT with $A_g = 0.1695$ and $T = 55$. The inset shows the linear fits giving $\delta^+$, $\delta^-$ and $\delta^0$(for more details see the text).

Fig. 4 – Critical curve $T_c$ vs. $A_{gc}$, showing the location of second-order IPTs driven by the oscillatory input between active regimes AR, trees+burning trees+empty sites) and the absorbing state (AS, only trees) in the FFMIT.

exponent $\delta$, as is shown in the inset of fig. 3. Our results, at criticality, are $\delta^+ \approx 0.46 \pm 0.02$, $\delta^- \approx 0.40 \pm 0.04$ and $\delta^0 \approx 0.43 \pm 0.03$, respectively. This finding suggests that $\delta^+ = \delta^0 = \delta^-$ considering both error bars and finite time corrections.

It is found that $R^2$ is less sensitive to the oscillatory input than $N(t)$ and $P(t)$. The plot of $R^2$ vs. $t$ can roughly be fitted by a straight line which yields a slope $z \approx 1.18 \pm 0.06$ (not shown here for the sake of space).

It should be noticed that the dynamic exponents which characterize the IPTs driven by the oscillatory parameter are in good agreement with those of the universality class of directed percolation (DP, in 2+1 dimensions), namely $\eta = 0.22295(10)$, $\delta = 0.4505(10)$, and $z = 1.1325(10)$ [14]. So, we conclude that the novel type of transition discussed so far can be placed in the universality class of DP. This result extends the validity of Janssen’s conjecture [15], which states that a continuous transition into an absorbing state characterized by a scalar order parameter may belong to the universality class of DP, to second-order irreversible transitions driven by oscillatory parameters.

Performing ES with different values of $A_g$ and $T$ we have evaluated the phase diagram of the FFMIT under oscillatory driving, as is shown in fig. 4. The critical curve $T_c$ vs. $A_{gc}$ shows the location of second-order IPTs between the active regimes (trees+burning trees+empty sites) and the absorbing state (only trees). All of these transitions belong to the universality class of DP.

Pointing our attention to the ZGB model, fig. 5 shows log-log plots of $N(t)$ vs. $t$ obtained by performing ES for a fixed period ($\tau = 20$ MCS) and different values of the amplitude $A_{PCO}$. In contrast to the FFMIT, here $N(t)$ decreases with time, as has been observed for ES at first-order IPTs [16]. Figure 5 also allows us to identify three regimes, $A_{PCO} = 0.123$ within the absorbing state, $A_{PCO} = 0.125$ at coexistence, and $A_{PCO} = 0.12345$ within the reactive
phase, respectively. While the ES of the second-order IPTs of the FFMIT exhibits power law behavior (fig. 2), the plot of fig. 5, at coexistence, exhibits marked curvature suggesting the crossover to a cut-off at certain long time. ES of the standard ZGB model at the first-order IPT shows a similar behavior [17]. Therefore, our results clearly point out that: i) the IPT driven by the oscillatory field in the ZGB model is of first order, and ii) the occurrence of power law (scale invariance) behavior can be ruled out. The latter finding agrees with the behavior of first-order reversible transitions, where it is well known that the existence of short-range correlations prevents the occurrence of scale invariance.

Performing ES of the ZGB model under oscillatory driving of the input parameter for different values of the period we have evaluated the corresponding phase diagram, namely a plot of $\tau_c$ vs. $A_{PCO}^c$, as is shown in fig. 6. The critical curve shows the location of first-order IPTs between a reactive state with CO$_2$ production and a poisoned inactive state where the catalyst’s surface is fully covered by CO. The inset of fig. 6 shows a log-log plot of $\tau_c$ vs. $\Delta A = A_{PCO}^c - (P_{2CO} - P_{CO})$. It is found that the data is consistent with a hyperbolic-like behavior $\tau_c \propto \Delta A^{\alpha}$ with exponent $\alpha \approx 1.53 \pm 0.01$. Although this scaling is presumably not genuine, it is interesting to note that the log-log plot allows to observe an interesting feature of the system, namely the fact that for short periods ($\tau_c < 1$), the value of the excess amplitude saturates just at $\Delta A_s = A_{PCO}^c / 2 = P_{2CO} - P_{CO} = 0.071$. This result can straightforwardly be interpreted assuming that such short periods are indeed much shorter than the relaxation time and consequently the system only feels the average value of the applied oscillatory pressure. Under these circumstances, the critical amplitude is expected to be $A_{PCO}^c = P_{CO}^w + 2\Delta A_s$, as has already been observed in fig. 6.

In summary, IPTs induced by an oscillatory external parameter are studied in two different systems, namely a forest fire model with immunity and a model for the catalytic oxidation
of carbon monoxide. Second-order IPTs are placed in the universality class of directed per-
colation in (2 + 1)-dimensions. However, first-order IPTs lack universal behavior. These
findings are in qualitative agreement with well-established concepts developed in the study of
reversible phase transitions. A phase diagram for this new type of IPTs is a critical curve,
period vs. amplitude of the oscillations, which sets the boundary between active regimes and
the absorbing state.

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