Entropy production as tool for characterizing nonequilibrium phase transitions

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(Dated: November 22, 2018)

Nonequilibrium phase transitions can be typified in a similar way to equilibrium systems, for instance, by the use of the order parameter. However, this characterization hides the irreversible character of the dynamics as well as its influence on the phase transition properties. Entropy production has revealed to be an important concept for filling this gap since it vanishes identically for equilibrium systems and is positive for the nonequilibrium case. Based on general arguments, we present distinct scenarios for the characterization of phase transitions in terms of entropy production. A full analysis is reported for discontinuous and continuous phase transitions; regular and complex topologies within the framework of mean field theory (MFT) and beyond the MFT. Our predictions will be exemplified by an icon system, perhaps the simplest nonequilibrium model presenting an order-disorder phase transition and spontaneous symmetry breaking: the majority vote model. Its dynamics is ruled by the misalignment and inertia parameters whose phase transition is continuous or discontinuous depending on symmetry, connectivity and inertia. Our work paves the way to a systematic description and classification of nonequilibrium phase transitions through a key indicator of system irreversibility.

Thermodynamics states that while certain quantities including the energy are ruled by a conservation law, the entropy is not conserved. In the general case of a system coupled with an environment, time variation of entropy \( dS/dt \) has two contributions: the flux to the reservoir \( \Phi \) and the entropy production \( \Pi \) component [1, 2] is given by

\[
\frac{dS}{dt} = \Pi(t) - \Phi(t).
\]  

(1)

Since in the steady state the time variation of \( S \) is null, \( dS/dt = 0 \), the entropy produced must be delivered to the environment. The entropy production properties have been subject of considerable interest in physics [3–7], population dynamics [8], biological systems [9], experimental verification [10] and others. A microscopic approach of entropy production broadly used is due to Schnakenberg [11]:

\[
\Pi(t) = \frac{k}{2} \sum_{ij} \{W_{ij}P_i(t) - W_{ji}P_j(t)\} \ln \frac{W_{ij}P_i(t)}{W_{ji}P_j(t)},
\]  

(2)

where \( W_{ij} \) is the transition rate from the state \( i \) to state \( j \) with associated probability \( P_i(t) \) at the time \( t \). Eq. (2) implies that \( \Pi(t) \) is always non negative because \((x - y)\ln(x/y) \geq 0\), vanishing when the detailed balance \( W_{ij}P_i - W_{ji}P_j = 0 \) is fulfilled. Thus it distinguishes equilibrium from nonequilibrium systems. Defining the nonequilibrium entropy by \( S(t) = -k \sum_i P_i(t) \ln P_i(t) \), a microscopic relation for the flux \( \Phi(t) \) can be obtained:

\[
\Phi(t) = \sum_j \Phi_j(t),
\]  

(3)

where \( \Phi_j(t) = k \sum_i W_{ij} \ln(W_{ij}/W_{ji})P_i(t) \). The steady state condition implies that \( \Pi = \Phi \) and Eq. (3) constitute an alternative approach for achieving the steady state condition implies that \( \Pi = \Phi \) and Eq. (3) constitutes an alternative approach for achieving the steady entropy production from the transition rates and it will be subject of analysis in the present Letter. A fundamental question is whether entropy production can be utilized as a reliable tool for typifying nonequilibrium phase transitions. In the last years, some studies have been undertaken [4, 7, 8, 12] in such direction, indicating that continuous phase transitions can be trademarked by a divergence of the first derivative of \( \Pi \) whose associated exponent plays an analogous role as the specific heat’s. However, all studies are restricted to critical phase transitions in regular topologies or mean-field analysis for particular examples.

Based on general arguments, we present distinct scenarios for the characterization of phase transitions in terms of entropy production. A full analysis is reported for discontinuous and continuous phase transitions in the framework of mean field theory (MFT) and beyond the MFT. Our work paves the way to a systematic description and classification of phase transitions through distinct entropy production hallmarks.

All theoretical findings will be exemplified in one of the simplest nonequilibrium phase transition model with steady states, the majority vote (MV) model [13, 14], defined as follows: Each site \( i \) of an arbitrary lattice can assume \( q \) possible integer values \( \sigma_i = 0, 1, ..., q - 1 \). The dynamics is ruled by the proportion \( \bar{w}_X \) of neighboring nodes in each one of the \( q \) states plus a local spin dependence \( \sigma_i \) (an inertial term), \( \bar{w}_{\sigma_i'} = (1 - \theta) \sum_{j=1}^{q} \delta(\sigma_i', \sigma_j)/k + \theta \delta(\sigma_i', \sigma_j) \), with \( \sigma_j \) denoting the spin of each one of the \( k \) nearest neighbors of the site \( i \). With probability \( 1 - f \) the local spin \( \sigma_i \) changes to the majority neighborhood spin \( \sigma_i' \) and with complementary probability \( f \) the majority rule is not followed. The MV is equivalent to the Ising model in contact with two heat reservoirs, one being a source of heat, at infinite temperature, and the other a sink of heat, at zero temperature [13]. Recent studies [15–17] revealed that large inertia shifts the phase transition to a discontin-
uous one for all values of $q$. An order-disorder phase transition arises by increasing the misalignment parameter $f$, whose classification depends on $\theta$ and the lattice connectivity $k$. For low $q$ ($q < 4$) and $\theta = 0$ (inertialless regime), it is always continuous [13–15], but the increase of $q$ modifies the symmetry properties ($Z_2$ and $C_{3\theta}$ for $q = 2$ and 3, respectively), leading to different sets of critical exponents. A given $n$–th order parameter moment $\langle m^n \rangle$ is calculated through the quantity $\langle m^n \rangle = (\sum_{i=1}^{N} e^{2\pi i n q / N})^{\frac{1}{n}}$, with (...) denoting the ensemble average. The $n = 1$ is a reliable order-parameter since $m > 0$ ($= 0$) in the ordered (disordered) phases. The entropy production is calculated from Eq. (3) through expression $\Pi = (\sum_{j=1}^{q-1} \sum_{i=1}^{N} w_i(\sigma) \ln[w_i(\sigma)/w_i(\sigma^j)]/N$ with $w_i(\sigma)$ and $w_i(\sigma^j)$ being the transition rate and its reverse, respectively. The latter is evaluated by taking transformation of $\sigma_j$ to one of its $q - 1$ distinct values. From now on, we will restrict ourselves to the case $q = 2$. Results for $q = 3$ will be presented in the Supplemental Material [22]. For $q = 2$, the transition rate above is more conveniently rewritten by taking the transformation $\sigma_j \rightarrow 2\sigma_j - 1$, so that $w_i(\sigma)$ and $m$ are rewritten as $w_i(\sigma) = \frac{1}{2}[1 - (1 - 2f)\sigma_i S(X)]$ and $m = (\sigma_i)$, respectively where $S(X)$ denotes the sign function evaluated over the local neighborhood plus the inertia $X = (1 - \theta) \sum_{j=1}^{q} \sigma_j / k + \theta \sigma_i$. The steady state expressions for the absolute $m$ and $\Pi$ then read $m = (1 - 2f)S(X)$ and

$$\Pi = \frac{1}{2} \ln \frac{\bar{f}}{1 - \bar{f}} \left[ \langle \sigma_i S'(X) \rangle - (1 - 2f) \langle S'^2(X) \rangle \right],$$

respectively where $S'(X)$ is the sign function evaluated only over local configurations in which $w_i(\sigma)/w_i(\sigma^j) \neq 1$. For the inertialless case, $S'(X) = S(X)$. Thus, the entropy production can be evaluated solely in terms of the averages $\langle S'(X) \rangle$ and $\langle S'^2(X) \rangle$. The simulation details, including the lattice topology and the dynamics are described in the Supplemental Material [22].

Analysis will be split out in four parts: discontinuous transitions in complex networks and regular lattices, continuous phase transitions and MFT. Distinct works [15–18] have attested that discontinuous phase transitions yield stark differences in regular and complex networks. In the former case, it emerges through sudden changes of $|m|$, its variance $\chi = N[\langle m^2 \rangle - |m|^2]$ and other quantities whose scaling behavior goes with the system volume $N$ (see e.g. panels (b)-(d) in Fig. 1). By appealing to the central limit theorem ideas, close to the transition the order-parameter probability distribution can be (approximately) written down as a sum of two independent gaussians, from which one extracts a scaling behavior with the system volume [17, 18]. Although $\Pi$ displays a non-trivial dependence on the system features and on generic correlations of type $(\sigma_i, (\sigma_j \sigma_{i+j})), (\sigma_i \sigma_{i+1} \sigma_{i+2})$ and so on, the generality of order-parameter distribution for tackling the phase coexistence [18] and Eq. (3) setting up $\Pi$ as an ensemble average suggest the extension of a similar relationship for the entropy production. More concretely, we assume that $P_N(\Pi) = P_N^{(a)}(\Pi) + P_N^{(b)}(\Pi)$, where $P_N^{(a)}(\Pi)$ is given by

$$P_N^{(a)}(\Pi) = \frac{\sqrt{N}}{2\pi} \exp[N(\Delta f - \Pi - (\Pi - \Pi_o)^2/(2\Pi_o))] / [F_o(\Delta f; N) + F_d(\Delta f; N)].$$

Each gaussian is centered at $\Pi_o$ with $\Delta f = f_0 - f_N$ corresponding to the width of the $\alpha$–th peak and the “distance” to the coexistence point $f_0$, respectively. Given that $P_N(\Pi)$ is normalized, each term $F_o(d)$ then reads $F_o(d)/\Delta f; N) = \sqrt{\chi_o(\Delta f)} / \chi_o(\Delta f) \exp \{ N \Delta f / [\Pi_o(d) + \chi_0(d) \Delta f/2] \}$. The entropy production $\Pi$ is straightforwardly calculated from $P_N(\Pi)$ distribution reading $\Pi = [F_o(\Delta f; N) + F_d(\Delta f; N)]^{-1} \sum_{\sigma = o(d)} (\Pi_o + \chi_o \Delta f) F_o(\Delta f; N)$ and can be approximately rewritten as

$$\Pi = \frac{\sqrt{\chi_o \Pi_o} + \sqrt{\chi_o \Delta f}}{\sqrt{\chi_o} + \sqrt{\chi_o \Pi_o} e^{-N(\Pi_o - \Pi_o) \Delta f}}$$

Note that the Eq. (5) reproduces the jump from $\Pi_o(\Pi_d)$ when $\Delta f \rightarrow 0_{+}$ and $N \rightarrow \infty$ (a third reason for assuming $P_N(\Pi)$ as a sum of independent gaussians). Remarkably, the curves for different values of $N$ cross at the transition point $\Delta f = 0$ with $\Pi'$ = $(\sqrt{\chi_0} + \sqrt{\chi_0 \Pi_o} + \sqrt{\chi_0 \Delta f})$. Fig. 1 exemplifies such predictions for the present model with $k = 20$ and $\theta = 0.375$ (see [17, 22] for simulation details). The intersection among curves (panels (a) and (b)) occurs at $f_0 = 0.05084(5)$, in excellent agreement with estimates 0.0509(1) (maximum of $\chi$), 0.0510(1) (minimum of $U_4 = 1 - (m^4)/(3 \langle m^2 \rangle^2)$), and 0.0509(1) (equal area order-parameter distribution $P_o(m)$) [18]-see e.g. panel (d). Collapse of all data by taking the transformation $y = (f - f_N) N$ (inset) reinforces the reliability of Eq. (5) describing $\Pi$ at the phase coexistence region. Out of the scaling regime ($f > f_0$ for large $N$), $\Pi$ depends solely on the control parameters ($f$ and $\theta$ for the MV), as can be seen in the upper inset of Fig. 1. The crossing in both order parameter and entropy production not only discerns the behavior from regular and complex topologies (see e.g. Fig. 2) but also discontinuous from continuous phase transitions (see e.g. Fig. 3). The generality of our findings is assured by attesting that the dependence on the system size comes from Eq. (5), which is valid for an arbitrary discontinuous phase transition, as can be viewed for $q = 3$ (Fig. 5 in [22]) and very recently for a catalytic surface reaction system [23].

In contrast to regular structures, the phase coexistence is akin to the MFT in complex networks (see e.g. Fig. 4), whose behavior is generally signed by the existence of a hysteretic loop and bistability [16, 24]. For locating the “forward transition” point $f_f$, the system is initially placed in an ordered configuration and the tuning parameter $f$ is increased by an amount $\Delta f$, whose final state at $f$ is used as the initial condition at $f + \Delta f$ until the order-parameter discontinuity is viewed. Conversely, the “backward transition” point $f_b$ is pinpointed by starting from the fully disordered phase and one decreases $f$.
Although the entropy production is finite in the critical point (panel (a)), $\Pi'$ increases without limits as $N \to \infty$.

Contrariwise, $\langle \sigma_i \sigma_{i+1} ... \sigma_{i+n} \rangle$ presents a nonzero well defined value in the ordered phase and $\Pi$ depends not only on the control parameters but also on correlations. So the order-parameter abruptly shifts at $f_f$ and $f_0$ will also be presented in the entropy production. The presence of bistability implies that $\Phi(t)$ will converge to one of two well definite values, since along the hysteretic branch the system behaves just like the disordered or ordered phase depending on the initial condition. Fig. 2 illustrates above trademark for the random-regular (RR) complex structures, with $k = 20$, $\theta = 0.3$ and $N = 10^4$. The hysteretic loop is located at the interval $f_0 < f < f_f$ (here with $f_0 = 0.055$ and $f_f = 0.15$). For larger inertia values (see inset and Fig. 5 in [22]), the bistability extends over $0 \leq f \leq f_f$. Fig. 4 from the Supplemental Material depicts, for both regular and complex topologies, the phase diagrams obtained from the entropy production signatures. As predicted, they are in full equivalence with those from the order-parameter analysis [15, 17]. It is worth mentioning that analogous findings are expected for phase transitions different from the order-disorder ones, provided the order-parameter and correlations also present a hysteretic behavior. Thereby, the entropy production behavior also embraces phase coexistence traits commonly treated in terms of the order-parameter.

Now we shift our analysis to critical phase transitions. Some works [4, 5] have argued that close to the criticality $\Pi$ and its first derivative $\Pi' \equiv d\Pi/df$ behave as $\Pi - \Pi_c \sim (f_c - f)^{-\alpha}$ and $\Pi' \sim (f_c - f)^{-\beta}$, with $\alpha$ and $\beta$ denoting their associated critical exponent respectively. Despite the continuity of $\Pi$, its derivative $\Pi'$ diverges at the transition. We will examine a novel case: random complex topologies. Albeit characterized by the order-parameter vanishment and algebraic divergences at the criticality, the behavior of quantities gets rounded due to finite size effects. According to the standard finite-size scaling (FSS), they behave as $|m| = N^{-\beta/\nu} f(N^{1/\nu}\epsilon)$, $\chi = N^{\gamma/\nu} g(N^{1/\nu}\epsilon)$ and more recently $\Pi' = N^{\alpha/\nu} \tilde{h}(N^{1/\nu}\epsilon)$, with $\tilde{f}$, $\tilde{g}$ and $\tilde{h}$ being scaling functions and $\epsilon$ denotes the “distance” to the critical point $\epsilon = (f - f_c)/f_c$. Typically, $f_c$ is located by identifying a proper quantity that intersect for distinct system sizes. In the present case, the quantity $U_4$ fulfills the requirement above whose crossing value $U^*_4$ depends on the lattice topology and the symmetry properties. Off the critical point and $N \to \infty$, $U_4 \to 2/3$ and 0 (for $q = 2$) in the ordered and disordered phases, respectively. Fig. 3 summarizes the results for RR structures. In that case, the critical behavior is consistent with the exponents $\beta/\nu = 1/4$, $\gamma/\nu = 1/2$ and $1/\nu = 1/2$ [MFT] and $\beta = 1/8$, $\gamma = 7/4$ and $1/\nu = 1$ (d = 2) [13]. Although the entropy production is finite in the critical point (panel (a)), $\Pi'$ increases without limits as $N \to \infty$.  

![Diagram 1](image1.png)

**FIG. 1.** Bidimensional lattice with $k = 20$ and $\theta = 0.375$. Panels (a)-(c) show the steady $\Pi$, the order parameter $|m|$ and the variance $\chi$ versus $f$, respectively for distinct system sizes at the vicinity of phase coexistence. Dashed lines: Crossing point among entropy production curves. Continuous lines in (a) and (b) correspond to the fittings from Eq. (5). Top and bottom insets: $\Pi$ for larger sets of $f$ and collapse of data by taking the relation $y = (f - f_0)N$, respectively. In (d), the plot of the maximum of $\chi$, minimum of $U_4$ and equal area order-parameter probability distribution versus $N^{-1}$.

![Diagram 2](image2.png)

**FIG. 2.** Panels (a) and (b) show the steady $\Pi$ and $|m|$ versus $f$ for $k = 20$, $\theta = 0.3$ for the random-regular (RR) case with $N = 10^4$. Black and red curves correspond to the forward and backward “trajectories”, respectively. Inset: The same but for $\theta = 0.375$. In (c) and (d), the time evolution of $\Phi(t)$ for distinct initial conditions $m_0$ for $f_0 < f_0 < f_f$ and $f = 0.20 > f_f$, respectively.
\[ m_0 < m_\infty^{(U)} \text{ and } m(t \to \infty) \to m_\infty^{(S)} \text{ if } m_0 > m_\infty^{(U)} \]

Since above phenomenological relations hide the irreversible character which we are interested, we derive a general expression for \( \Pi \) taking into account a generic \( Z_2 \) symmetry transition rate \( w(\sigma) = \frac{1}{2}(1 - g(\sigma g(X))) \), where \( g(X) \) expresses an arbitrary dependence on the local neighborhood. Using the results detailed in the Supplemental Material [22], one-site mean-field theory (MFT) predicts a jump in the first derivative of \( \Pi \) at the criticality, from which one associates the exponent \( \alpha = 0 \). From the above, we see that the hyperscaling relation \( \alpha = \beta + \gamma = 2 \) is again satisfied, reinforcing that the criticality is signed by the jump in the first derivative of \( \Pi \), in close similarity to the specific heat discontinuity for equilibrium systems. Instead, discontinuous transitions are featured by a hysteric loop in \( \Pi \). Below we show explicit results for \( \Pi \) when \( q = 1 - 2f \) and \( g(X) = S'(X) \). In such case, \( \Pi = \ln[f/(1 - f)](m(S'(X)) - (1 - 2f)(S'(X)^2))/2 \), with \( (S'(X)) \) and \( (S'(X)^2) \) depending only on \( f, \theta, k \) and \( m \) (see [22] for more details). Above equation can also be obtained from Eq. (4) by replacing \( \langle \sigma, S'(X) \rangle \) for \( \langle \sigma, S'(X) \rangle \). In terms of the order parameter, the phase transition is discontinuous for larger \( k \)'s when \( \theta \) goes up [see e.g. Fig. 4 for \( k = 12 \)] and continuous for low \( \theta \) [see e.g Fig. 5]. As in complex structures, \( \Phi(t) \) also converges to two well defined values of \( \Pi \) and \( \Pi_0 \equiv \Pi(m_\infty^{(S)}, f, \theta) \) in the region \( f_b < f < f_f \). Such theoretical predictions have been very recently verified in a catalytic surface reaction system, reinforcing the generality of our description [23].

FIG. 4. Panel (a) depicts the bistable behavior of \( \Pi \) for \( \theta = 0.43 \) and \( k = 12 \). Black (blue) curves denote the stable solutions for \( m_0 > m_\infty^{(U)} \) (\( m_0 < m_\infty^{(U)} \)). They coincide themselves for \( f > f_f \) and \( f < f_b \) and are different for \( f_b < f < f_f \). The red curves correspond the unstable solutions for \( f_b < f < f_f \) with \( m = m_\infty^{(U)}(f) \) if \( m_0 = m_\infty^{(U)} \). Inset: The same but for the order-parameter. In (b) the time evolution of flux \( \Phi(t) \) for distinct initial configurations and \( f = 0.078 \). Inset: The time evolution of \( m(t) \), where circles correspond to the function \( m(t) \sim e^{m(f - f_\infty)t} \), valid for \( m_0 << 1 \).
FIG. 5. Left and right panels: Steady entropy production $\Pi$ and its derivative $\Pi'$ versus $f$ for low $\theta$, $k = 4$ (top) and $k = 12$ (bottom), respectively. Inset: The corresponding order parameter versus $f$. Dashed lines denote the associated critical points.

$\Pi$ acquire simpler expressions $m = (1 - 2f)\text{erf}(m\sqrt{k/2})$ and $\Pi = \frac{1}{2} \ln f \left[ \frac{m^2}{1 + f} - (1 - 2f) \right]$, respectively whose critical point reads $2f_{\text{c}} = \left\{ 1 - \sqrt{(\pi/2k)} \right\}$. Close to $f \rightarrow f_{\text{c}}$, they behave as $m \sim A(f_{\text{c}} - f)^{1/2}$ (with $A^2 = 12/k$) and $\Pi \approx \frac{1}{2} \ln f \left[ 1 - \frac{12}{k} \frac{f_{\text{c}} - f}{(1 - 2f)\pi} \right]$ respectively. For $f > f_{\text{c}}$, $\Pi = \frac{1}{2} \ln f$ and thereby the order-parameter vanishment is followed by a (continuous) peak in the entropy production. Notwithstanding, $\Pi'$ jumps from $\frac{1}{2} \sqrt{\pi k} \ln \frac{1 + \sqrt{\pi k}}{1 - \sqrt{\pi k}} \approx \frac{12}{k} \ln \frac{1 + \sqrt{\pi k}}{1 - \sqrt{\pi k}}$ at the criticality, consistent with $\alpha_{mf} = 0$ (see e.g. panels (b) and (d)). By increasing $\theta$ (see e.g $\theta = 0.4$ and 0.3 for $k = 4$ and $k = 12$ for respectively), the maximum of $\Pi$ does not coincide with the jump of $\Pi'$. Thereby the present work also unifies the description in the MFT context, in which the criticality is not necessarily marked by a peak in the entropy production but related to a peculiar behavior its first derivative.

We presented the analysis of entropy production for the characterization of nonequilibrium phase transitions. Based on general arguments, continuous and discontinuous phase transitions can be classified through distinct entropy production traits in the realm of mean-field theory and beyond the MFT. Our work is a relevant step in trying to unify the description of nonequilibrium phase transitions through a key indicator of system irreversibility.

[1] I. Prigogine, *Introduction to Thermodynamics of Irreversible Processes*, 2nd ed. (Wiley, New York, 1961).
[2] S. R. de Groot and P. Mazur, *Non-Equilibrium Thermodynamics* (North-Holland, Amsterdam, 1962).
[3] U. Seifert, Rep. Prog. Phys. **75**, 126001 (2012).
[4] L. Crochik and T. Tomé, Phys. Rev. E **72**, 057103 (2005).
[5] T. Tomé and M. J. de Oliveira, Phys. Rev. Lett. **108**, 020601 (2012).
[6] T. Tomé and M. J. de Oliveira, Phys. Rev. E. **91**, 042140 (2015).
[7] Y. Zhang and A. C. Barato, J. Stat. Mech. **2016**, 113207 (2016).
[8] B. Andrae, J. Cremer, T. Reichenbach and E. Frey, Phys. Rev. Lett. **104**, 218102 (2010).
[9] D. Mandal, K. Klymko and M. R. DeWeese, Phys. Rev. Lett **119**, 258001 (2017).
[10] M Brunelli, L. Fusco, W. Wieczorek, J. Hoelscher-Obermaier, G. T. Landi, F. L. Semio, A. Ferraro, N. Kiesel, T. Donner, G. De Chiara and M. Paternostro, Phys. Rev. Lett **121**, 16064 (2018).
[11] J. Schnakenberg, Rev. Mod. Phys. **48**, 571 (1976).
[12] A. C. Barato and H. Hinrichsen, J. Phys. A **45**, 115005 (2012).
[13] M. J. de Oliveira, J. Stat. Phys. **66**, 273 (1992).
[14] H. Chen, C. Shen, G. He, H. Zhang and Z. Hou, Phys. Rev. E **91**, 022816 (2015).
[15] H. Chen, C. Shen, H. Zhang, G. Li, Z. Hou and J. Kurths, Phys. Rev. E. **95**, 042304 (2017).
[16] P. E. Harunari, M. M. de Oliveira, and C. E. Fiore, Phys Rev E **96**, 042305 (2017).
[17] J. M. Encinas, P. E. Harunari, M. M. de Oliveira and C. E. Fiore, Sci. Rep. **8**, 9338 (2018).
[18] M. M. de Oliveira, M. G. E. da Luz and C. E. Fiore, Phys. Rev. E **97**, 060101(R) (2018).
[19] R. Zieren, A. Maritan and H. Hinrichsen, J. Stat. Mech. **2015**, P08014 (2015).
[20] L. F. Pereira and F. G. B. Moreira, Phys. Rev. E **71**, 016123 (2005).
[21] B. Bollobás, *Europ. J. Combinatorics*, **1**, 311 (1980).
[22] Supplemental Material, where additional details on the formal aspects of our investigation are given.
[23] M. Pineda and M. Stamatakis, Entropy **20**, 811 (2018).
[24] See e.g. J. Gómez-Gardeñes, S. Gómez, A. Arenas and Y. Moreno, Phys. Rev. Lett. **106**, 128701 (2011).
I. ENTROPY PRODUCTION AND MFT

A. General behavior for $Z_2$ symmetry

Take for instance an arbitrary dynamics with $Z_2$ symmetry in which each site $i$ is attached to a spin variable $\sigma_i$ that assumes the values $\pm 1$. The transition rate is given by the generic expression $w(\sigma_i) = \frac{1}{2}[1 - q\sigma_i g(X)]$, with $q$ denoting the control parameter and $g(X)$ expressing the generic dependence on a local neighborhood of $k$ spins. Only two assumptions regarding $g(X)$ are required. The former is that due to the $Z_2$ symmetry, it depends on the signal of the local spin neighborhood (odd function). Also, taking into account that $w(\sigma_i)$ is constrained between 0 and 1, $g(X)$ should be limited for all values of $X$. These points allow us to rewrite $g(X)$ as $g(X) = |g(X)|S(X)$, where $S(X)$ denotes the sign function: $\text{sign}(X) = 1(-1)$ and 0, according to $X > 0(<0)$ and $X = 0$, respectively where $|g(X)|$ gets restricted between 0 and $|g(k)|$.

The time evolution of order parameter $m = \langle \sigma_i \rangle$ is given by

$$\frac{d}{dt} \langle \sigma_i \rangle = -2\sigma_i w(\sigma_i),$$

(1)

whose steady state satisfy the relation $m = q\langle |g(X)| S(X) \rangle$. For the achievement of $\Pi$, it is required the calculation of $[w_i(\sigma_i)/w_j(\sigma_j)]\ln[w_i(\sigma_i)/w_j(\sigma_j)]$ given by

$$\frac{1}{2} \left[ \sigma_i S(X) - q \langle |g(X)| S(X) \rangle \left| S(X) \right| \ln \frac{1 - q \langle |g(X)| \rangle}{1 + q \langle |g(X)| \rangle} \right].$$

(2)

The one-site MFT consists of rewriting the joint probability $P(\sigma_1, \ldots, \sigma_{i+k})$ as a product of one-site probabilities $P(\sigma_1) \ldots P(\sigma_{i+k})$, from which one derives closed relations for all model properties as function of the control parameters. Since the main marks of critical and discontinuous phase transitions are expected not depending on the particularities of $g(X)$, it is reasonable, within the mean-field approximation, to replace the averages in terms of an effective $\tilde{g}$ given by $q\langle |g(X)| S(X) \rangle \to q\tilde{g}\langle S(X) \rangle$,

$$\frac{1}{2} \left[ \sigma_i S(X) - q \tilde{g} \langle S(X) \rangle \right] \ln \frac{1 - q \tilde{g} \langle S(X) \rangle}{1 + q \tilde{g} \langle S(X) \rangle} \to \frac{1}{2} \left[ \sigma_i S(X) - q \tilde{g} \langle S(X) \rangle \right] \ln \frac{1 - q \tilde{g} \langle S(X) \rangle}{1 + q \tilde{g} \langle S(X) \rangle},$$

(3)

and

$$\frac{1}{2} \left[ \langle g(X) \rangle S^2(X) - q \tilde{g} \langle S(X) \rangle \right] \ln \frac{1 - q \tilde{g} \langle S(X) \rangle}{1 + q \tilde{g} \langle S(X) \rangle} \to \frac{1}{2} \left[ \langle g(X) \rangle S^2(X) - q \tilde{g} \langle S(X) \rangle \right] \ln \frac{1 - q \tilde{g} \langle S(X) \rangle}{1 + q \tilde{g} \langle S(X) \rangle}.$$

(4)

At this level of approximation the steady $\Pi$ then reads

$$\Pi = \frac{1}{2} \ln \left[ \frac{1 - q \tilde{g}}{1 + q \tilde{g}} \frac{m \langle S(X) \rangle - q \tilde{g} \langle S^2(X) \rangle}{m \langle S(X) \rangle + q \tilde{g} \langle S^2(X) \rangle} \right].$$

(5)

Above averages are calculated by decomposing the mean sign function in two parts $\langle S(X) \rangle = \langle S(X_+) \rangle - \langle S(X_-) \rangle$, with each term being approximated by

$$\langle S(X_\pm) \rangle \approx \pm \sum_{n=|n_\pm|}^k C^k_n p^k_\pm p^k_{-n},$$

(6)

where $[n_\pm]$ denote the lower limits in the ceiling function and for $\langle S(X_+) \rangle [\langle S(X_-) \rangle ]$ the term $C^k_n$ takes into account the number of possibilities of a neighborhood with $n$ and $k - n$ spins in the $+1[-1]$ and $-1[+1]$ states with associated probabilities $p_\pm = (1 \pm m)/2$. In the regime of large connectivities, $\langle S(X_\pm) \rangle$ acquires a simpler way in which each term from the binomial distribution approaches to a gaussian one with mean $kp_\pm$ and variance $\sigma^2 = kp_\pm p_{-n}$, whereas $\langle S^2(X) \rangle \to 1$. Thus, the expression for $\Pi$ becomes

$$\Pi = \frac{1}{2} \ln \left[ \frac{1 - q \tilde{g}}{1 + q \tilde{g}} \frac{m^2 - q \tilde{g}}{m^2 + q \tilde{g}} \right].$$

(7)

Since at the vicinity of the critical point $m$ behaves $m \sim (q - q_c)^{1/2}$, the entropy production is continuous at $q_c$, $\Pi_c = \frac{q_c^2}{2} \ln \frac{1 + q_c^2}{1 - q_c^2}$. However, its first derivative is discontinuous, jumping from $\Pi' = \frac{1}{4} \left( \ln \frac{1 - q_c^2}{1 + q_c^2} - \frac{1}{2} \ln \frac{1 - q_c^2}{1 + q_c^2} \right)$ to $\Pi'' = \frac{1}{4} \ln \frac{1 - q_c^2}{1 + q_c^2}$, whose discontinuity of $\frac{q_c^2}{2} \ln \frac{1 - q_c^2}{1 + q_c^2}$ is associated with the critical exponent $\alpha_{mf} = 0$.

The simplest approach used to study a discontinuous phase transition is described and understood in terms of the logistic equation $dm/dt = a(q - m)m - bm^3 + cm^5$ (with $c > 0$) [1, 2]. At $q = q_f = (b^2/4ac) - q_0$, $m$ jumps from $m_1 \equiv m_\infty(S(q_f))$ to 0. The value $q = q_0$ separates the exponential vanishing of $m \sim e^{(q_0 - q)^n}$ ($q > q_0$) from the convergence to a well defined $m_2 \equiv m_\infty(q)$ ($q < q_0$) when $m_0 << 1$. Along the hysteretic branch, $q_0 < q < q_f$, the steady $m_\infty$ will depend on the initial configuration $m_0$ (see main text for a more detailed discussion).

All these upshots can alternatively be portrayed in terms of the entropy production and Eq. (7) also predicts correctly the bistability. At $q = q_f$, $\Pi$ jumps from $\ln[1 + (2q_q)g]/(1 - (2q_q)g)$ to $\ln[1 + (2q_q)/2 - (m_q^2/2q_qg)]$, whereas at $q = q_0$, $\Pi$ jumps from $\ln[1 + (2q_q)g]/(1 - (2q_q)g)$ to $\ln[1 + (2q_q)g]/[2 - (m_q^2/2q_qg)]$. 

Dated: November 22, 2018

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Supplemental Material for “Entropy production as tool for characterizing nonequilibrium phase transitions”
B. Majority Vote model

In this subsection we illustrate all above predictions for majority vote model, corresponding to the particular case \( q = 1 - 2f \), \( g(X) = S(X) \) with \( X \) given by \( X = (1 - \theta) \sum_{j=1}^{k} \sigma_j / k + \theta \sigma_i \). The transition rate and the MFT expression for \( m \) read \( w(\sigma_i) = \frac{1}{2} (1 - 1 - (1 - 2f) \sigma_i S(X) \) and

\[
m = (1 - 2f) \left[ \frac{1}{2} (1 + m) - \frac{1}{2} (1 - m) \right],
\]

respectively. In the regime of large \( k \), Eq. (8) becomes

\[
m = \frac{(1 - 2f)}{2} \frac{\text{erf}(a) - \text{erf}(b)}{\text{erf}(a) + \text{erf}(b)},
\]

where \( \text{erf}(x) \) denotes the error function, with \( a \) and \( b \) given by \( a = \sqrt{(k/2)[\theta/(1 - \theta) + m]} \) and \( b = \sqrt{(k/2)[\theta/(1 - \theta) - m]} \), respectively. For \( \theta = 0 \) it reduces to the expression \( m = (1 - 2f) \text{erf} \left[ m \sqrt{k/2} \right] \), whose critical point is located at \( 2f_c = 1 - \sqrt{\pi/(2k)} \). At the vicinity of \( f_c \), \( m \) behaves as \( m \sim A(f_c - f)^{\delta_{mf}} \), with \( \delta_{mf} = 1/2 \) (as expected) and \( A^2 = 12/k \).

By repeating the previous calculations for \( \Pi \) we have that

\[
\frac{w_i(\sigma)}{w_i(\sigma')} = \frac{1 - (1 - 2f) \sigma_i S(\sum_{j=1}^{k} \sigma_j + \frac{k \theta}{1 - \theta} \sigma_i)}{1 + (1 - 2f) \sigma_i S(\sum_{j=1}^{k} \sigma_j - \frac{k \theta}{1 - \theta} \sigma_i)}. \tag{10}
\]

Inspection of Eq. (10) reveals that only local configurations with \( |\sum_{j=1}^{k} \sigma_j| \) greater than \( \frac{k \theta}{1 - \theta} \) will contribute for \( \Pi \), since only in those cases the ratio is different from 1. Thus, it can be rewritten as \( w_i(\sigma)/w_i(\sigma') = \sigma_i S'(X) \text{ln} \frac{f_1}{f_2} \), with \( S'(X) \) being the sign function evaluated only over the subspace of local configurations in which the ratio is different from 1. For \( \theta = 0 \), it reduces to the usual sign function. Thus \( \Pi \) and its mean-field expression are given by

\[
\Pi = \frac{1}{2} \ln \frac{f}{1 - f} \left[ (\sigma_i S'(X)) - (1 - 2f) (S'^2(X)) \right], \tag{11}
\]

and

\[
\Pi = \frac{1}{2} \ln \frac{f}{1 - f} \left[ m(S'(X)) - (1 - 2f) (S'^2(X)) \right]. \tag{12}
\]

respectively. In Fig. 1 we plot the phase diagrams for \( k = 12 \) and \( k = 20 \) evaluated by means of distinct entropy production signatures. We see that both phase transition location and its classification are in full agreement with those obtained from order-parameter analysis (see e.g. Refs. [2, 3]).

A remarkable particular case is the complete graph regime \( (k \rightarrow \infty) \) with \( m \) and \( \Pi \) given by

\[
m = \frac{(1 - 2f)}{2} \frac{S(\frac{\theta}{1 - \theta} + m) - S(\frac{\theta}{1 - \theta} - m)}{S(\frac{\theta}{1 - \theta} + m) + S(\frac{\theta}{1 - \theta} - m)}, \tag{13}
\]

and

\[
\Pi = \ln \frac{f}{1 - f} \left[ m - (1 - 2f) Y_p \right], \tag{14}
\]

respectively, where \( Y_p = \{(1 + m) S[m + \theta/(1 - \theta)] - (1 - m) S[m - \theta/(1 - \theta)]\} / 2 \). Above expression is strictly null since \( Y_p = m/(1 - 2f) \) [from Eq. (13)], implying that there is no entropy production in complete graph case. The reversible character of the inertialess MV in the complete graph has already been presented in Ref. [4] and our analysis not only confirms it but also extends for the inertial regime.

II. NUMERICAL SIMULATIONS

Random regular networks have been generated through a configuration model scheme [5] described as follows: For a system with \( N \) nodes and connectivity \( k \), we first start with a set of \( Nk \) points, distributed in \( N \) groups, in which each one contains exactly \( k \) points. Next, one chooses a random pairing of the points between groups and then creates a network linking the nodes \( i \) and \( j \) if there is a pair containing points in the \( i \)-th and \( j \)-th sets until \( Nk/2 \) pairs (links) are obtained. If the resulting network configuration present a loop or duplicate links, the above process is restarted. Bidimensional topologies with a given connectivity \( k \) forms a regular arrangement, whose increase of connectivity is accomplished by extending the range of interaction neighborhood. For example, \( k = 4, 8, 12 \) and 20 includes interaction between the first, first and second, first to third and first to fourth next neighbors, respectively, as sketched in Fig. 2. All studied structures are quenched, i.e., they do not change during the simulation of the model. For a given network topology, \( N \), \( f \), and \( \theta \) held fixed, a site \( i \) is randomly chosen,
and its spin value $\sigma_i$ is updated ($\sigma_i \rightarrow \sigma_i'$) according to
\[ \bar{w}_{\sigma_i'} = (1 - \theta) \sum_{j=1}^{k} \delta(\sigma_i', \sigma_j)/k + \theta \delta(\sigma_i', \sigma_i), \]
with $\sigma_j$ denoting the spin of each one of the $k$ nearest neighbors of the site $i$. With probability $1 - f$, $\sigma_i$ changes to the majority neighborhood spin $\sigma_i'$ and with complementary probability $f$ the majority rule is not followed.

A Monte Carlo (MC) step corresponds to $N$ updating spin trials. After repeating the above dynamics a sufficient number of MC steps (in order of $10^6$ MC steps), the system attains a nonequilibrium steady state.

![FIG. 2. Local configuration for a bidimensional lattice with central site (red) and its first (1), second (2), third (3) and fourth (4) next neighbors.](image)

### A. The $q = 2$ case

In contrast to the RR case, the inclusion of inertia does not shift the phase transition to a discontinuous one nor change the critical behavior when $k < 20$, irrespective the inertia strength [2]. Fig. 3 illustrates that this finding, commonly viewed in terms of the order-parameter, can also be achieved through entropy production $\Pi$ and its derivative $\Pi'$ features.

Fig. 4 depicts the phase diagrams for $k = 20$ (the $k = 12$ case is analogous, but no coexistence line is presented in regular lattices). Continuous and discontinuous phase transitions are identified through the aforementioned features. As expected, all transition points calculated through entropy production analysis are equivalent to those from the order-parameter [2].

### B. Discontinuous transitions for $q = 3$

We analyze the properties of MV with $q = 3$ in which the $C_{3v}$ symmetry leads to an entirely different critical behavior from the $q = 2$ case. Figs. 5 and 6 depict the main results for the bidimensional and random-regular structures for $k = 20$.

Analysis of entropy production trademarks at the phase coexistence are very similar to $q = 2$ ones, including the existence of bistability (complex networks), crossing among curves at the transition point ($f_0 = 0.14160(5)$) and scaling with the system volume (regular structures), thereby reinforcing the robustness of our findings at discontinuous phase transitions.

![FIG. 3. Regular lattice for interactions between the first to the third next neighbors ($k = 12$) and $\theta = 0.2$: Panels (a), (b) and (c) depict the entropy production $\Pi$, its derivative $\Pi'$ the variance $\chi$ versus $f$, respectively for distinct system sizes. Inset: The same but for fourth-order reduced cumulant $U_4$. Dashed lines denote the critical point $f_c$ evaluated through the crossing among $U_4$ curves. In (d), the $\ln \chi_N$, $\ln |m|_{N}$ and $\Pi'_N$ versus $\ln N$ at $f = f_c$.](image)

![FIG. 4. Panels (a) and (b) show the phase diagrams for $k = 20$ for regular and RR structures, respectively through analysis of entropy production. ORD (DIS) denote the ordered (disordered) phases and continuous (dashed) lines correspond to continuous and discontinuous phase transitions, respectively. In (b), circles (x) correspond to the increase (decrease) of $f$ starting from an ordered (disordered) phase.](image)
FIG. 5. Regular lattice for $k = 20$ and $\theta = 0.32$: Panels (a)-(c) depict the steady $\Pi$, the order parameter $|m|$ and the variance $\chi$ versus $f$, respectively for distinct system sizes at the vicinity of phase coexistence. Dashed lines: Crossing point among entropy production curves. Continuous lines in (a) and (b) are the fittings from Eq. (6) (see main text). Inset: Collapse of data by taking the relation $y = (f - f_0)N$. In (d), the plot of the maximum of $\chi$ versus $N^{-1}$.

FIG. 6. For the RR structure, panels (a) and (b) show the steady $\Pi$ and $|m|$ versus $f$ for $k = 20$ and $\theta = 0.35$. In (c) and (d), the time evolution of $\Phi(t)$ for distinct initial conditions for $f = 0.15$ (bistable loop) and $f = 0.25$ (disordered phase), respectively.

[1] See e.g. P. V. Martín, J. A. Bonachela, S. A. Levin, and M. A. Muñoz, Proc. Natl. Acad. Sci. USA 112, E1828 (2015).
[2] J. M. Encinas, P. E. Harunari, M. M. de Oliveira, and C. E. Fiore, Sci. Rep. 8, 9338 (2018).
[3] H. Chen, C. Shen, H. Zhang, G. Li, Z. Hou and J. Kurths, Phys Rev. E 95, 042304 (2017).
[4] A. Fronczak and P. Fronczak, Phys. Rev. E 96, 012304 (2017).
[5] B. Bollobás, Europ. J. Combinatorics. 1, 311 (1980).