# Generic finite size scaling for discontinuous nonequilibrium phase transitions into absorbing states

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Based on quasistationary distribution ideas, a general finite size scaling theory is proposed for discontinuous nonequilibrium phase transitions into absorbing states. Analogously to the equilibrium case, we show that quantities such as response functions, cumulants, and equal area probability distributions all scale with the volume, thus allowing proper estimates for the thermodynamic limit. To illustrate these results, five very distinct lattice models displaying nonequilibrium transitions—to single and infinitely many absorbing states—are investigated. The innate difficulties in analyzing absorbing phase transitions are circumvented through quasistationary simulation methods. Our findings (allied to numerical studies in the literature) strongly point to a unifying discontinuous phase transition scaling behavior for equilibrium and this important class of nonequilibrium systems.

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## I. INTRODUCTION

A nonequilibrium phase transition (NEQPT) into absorbing states (AS) is key in a wide range of phenomena, such as [1–5] chemical reactions, interface growth, epidemics, and population dynamics. Likewise, it is relevant for the emergence of spatiotemporal chaos in different classes of problems, as experimentally verified in liquid crystal electroconvection [6], driven suspensions [7], and superconducting vortices [8]. So, much has been done on continuous NEQPT, especially addressing universality [3,5,9,10]. However, comparatively less attention has been paid to *discontinuous* transitions in systems with AS [11,12], the case, e.g., in catastrophic shift processes [13] (bearing important questions regarding the influence of diffusion and disorder in creating or destroying AS), heterogeneous catalysis [14,15], ecological [16,17], granular [18], and replicator dynamics [19], cooperative coinfection [20], language formation [21], and social patterns [22].

Discontinuous transitions to AS conceivably require mechanisms to suppress the formation of absorbing minority islands induced by fluctuations [23,24]. Also, there is strong evidence that they cannot occur in one dimension (1D) if the interactions are short ranged: The absence of boundary fields would prevent the stabilization of compact clusters [25]. In spite of these presumably universal facts, a general description of discontinuous NEQPT, including the ability to identify a possible scaling behavior, is still lacking.

Equilibrium first-order transitions are characterized by discontinuities in the order parameter $\phi$ and by thermodynamic "densities", whose susceptibilities display deltalike shapes. In finite systems, such quantities become continuous functions of the control parameter $\lambda$. However, the infinite limit still can be estimated from a finite size scaling theory (FSS) [26–33], when second derivatives scale linearly with the volume $V = L^d$ (for $d$ the spatial dimension and $L$ the lattice size). Also, $|\lambda_V - \lambda_0|$ goes with $1/V$, with $\lambda_V$ ($\lambda_0$) the coexistence point for a finite $V$ (in the thermodynamic limit).

For NEQPT to AS, precise methods such as spreading simulations—available for continuous transitions—as well as a FSS framework (as the above) are absent in the discontinuous case. Actually, a difficulty in its analysis is that the AS often prevent simulations to properly converge, precluding any scaling inference. Even for large systems, eventually the dynamics will end up in an AS via a statistical fluctuation of small, but nonzero, probability. Also, metastable states can make it hard to locate or even classify transition points due to doubts if the observed order parameter jump is genuine.

In the present article we address such a class of problems, presenting solid arguments for a common finite size scaling behavior. Based on previous suggestions [11,34–36]—and in the fact that equilibrium and nonequilibrium phase transitions share important similarities when the latter display stationary (steady) states [37] (see below)—we develop a FSS for transitions into single and infinitely many AS by means of the quasistationary (QS) concept. We show that, in full analogy with equilibrium, standard quantities follow the same $1/V$ scaling. Five models are used to illustrate our results.

## II. THEORY AND METHOD

The quasistationary probability distribution (QSPD) idea, powerful for continuous NEQPTs [38], is likewise valuable here. In very general terms, the main purpose of such a method is to evade just the absorption process. Formally, assume at time $t$ the microstate ($\sigma$) probability distribution $P(\sigma,t)$ and the survival probability $P_s(t)$, i.e., the probability that the system is still active. Then, the QSPD, $P_{\rm QS}(\sigma) = \lim_{t\to\infty} P(\sigma,t)/P_s(t)$, describes the asymptotic properties of a finite system conditioned to survival [39,40]. In practice, $P_{\rm QS}$ is calculated by effectively redistributing the flux from the absorbing state to the system's nonabsorbing subspace when the dynamics is sufficiently close to the absorbing condition. In this case, although the detailed balance is not satisfied, if the redistribution is made compatible with the QS distribution itself (through a self-consistent procedure—see Ref. [38]), then the global balance [41] is verified in the nonabsorbing subspace of the original problem. Furthermore, the QS distribution becomes the stationary solution of the

 

modified process [39]. Thus, typical quantities in a QS ensemble usually converge to the corresponding stationary ones when $L \to \infty$ [39].

For no spatial structure problems, analytic QSPDs have been obtained from the master equation. Indeed, for some discontinuous transitions, including Schlögl (second) [42] and Ziff-Gulari-Barshad (ZGB) [14] models, a mean field calculation [39,43] resulted in bimodal QSPDs. Nevertheless, to portray QSPDs for systems with spatial structures, one must rely on numerical protocols. An efficient scheme is that given in Ref. [38], which stores and gradually updates a set of configurations (compatible with the QS ensemble) visited during the time evolution. Whenever a transition to AS is imminent, the system is "relocated" to one of the saved configurations. This accurately reproduces the results from the much longer procedure of performing averages only on samples that have not visited the AS at the end of their respective runs.

To construct a FSS for discontinuous NEQPTs to AS, we now observe the following. First, the role of inverse flux is to turn off the system's natural sink, thus with the absorbing becoming a "usual" phase [but with most of its dynamics still properly taken into account through $P(\sigma,t)$—see the expression for $P_{\rm QS}$ above]. Second, certainly the resulting effective problem does not become reversible, but it has a weaker nonequilibrium character, presenting steady states (the global balance, restored by the inverse flux, guarantees this latter fact [44]). Third, we can always associate a stable probability density to a nonequilibrium steady state [45]. Very importantly, such a stationarity allows an extended version of the central limit theorem to hold true. So, the corresponding distribution can be described by Gaussians [46].

As already mentioned, in the thermodynamic limit [39] we can expect this recipe to effectively and fairly reproduce the macroscopic transition behavior of the original system. Moreover, it represents a discontinuous transition between two "normal" phases $\pm$, bearing two scales, the order parameter $\phi = \phi_\pm$ at the transition point. Hence, in general, for a finite but nonetheless reasonably large $V$, the bimodal probability distribution is reasonably well described by a sum of two Gaussians (see Refs. [27–30]) $P_V(\phi) = \sum_{\omega=\pm} P_V^{(\omega)}(\phi)$, with $(\tilde{\lambda} = \lambda - \lambda_0)$

$$P_V^{(\omega)}(\phi) = \frac{\sqrt{V}}{\sqrt{2\pi}} \frac{\exp[g(V)\tilde{\lambda}\phi - g(V)(\phi-\phi_\omega)^2/(2\chi_\omega)]}{[F_-(\tilde{\lambda};V) + F_+(\tilde{\lambda};V)]}. \tag{1}$$

$\lambda_0$ is the control parameter value at the phase transition in the thermodynamic limit, the $F$'s give the normalization, and $g(V)$ is an increasing function of $V$. $P_V(\phi)$ has the expected behavior: For $V \to \infty$ and $\lambda = \lambda_0$, we get the superposition of two $\delta$ functions centered at $\phi = \phi_\pm$. For the extensive case $g(V) = V$,

$$F_\pm(\tilde{\lambda};V) = \sqrt{\chi_\pm}\exp\left[V\tilde{\lambda}\left(\phi_\pm + \frac{\chi_\pm}{2}\tilde{\lambda}\right)\right]. \tag{2}$$

Now, the pseudotransition point $\lambda_V$ can be estimated, e.g., from (i) the coexisting phase equal probability condition, i.e., equal areas of $P_V^{(-)}$ and $P_V^{(+)}$, or yet from the maximum of (ii) variance $\chi = V(\langle\phi^2\rangle - \langle\phi\rangle^2)$, and (iii) the moment ratio (reduced cumulant) $U_2 = \langle\phi^2\rangle/\langle\phi\rangle^2$. In first order in $\tilde{\lambda}$ [47], both (i) and (ii) lead to $\lambda_V = \lambda_0 - V^{-1}\ln[\chi_+/\chi_-]/[2(\phi_+ + \phi_-)]$. For (iii), we get $\lambda_V = \lambda_0 - V^{-1}(\ln[\chi_-/\chi_+] + 2\ln[\phi_-/\phi_+])/[2(\phi_- - \phi_+)]$. Note that $|\lambda_V - \lambda_0|$ is the same if it is estimated via equal areas or the maximum of $\chi$, and does not differ too much if derived by the $U_2$ maximum. Thus, distinct measures show that $|\lambda_V - \lambda_0| \sim 1/V$, the usual equilibrium scaling.

This description is illustrated by periodic square lattice models simulated from the QS approach. For the equal area criterion, whenever $P_V^{(\pm)}(\phi)$ have a relevant overlap, we consider each $P_V^{(\omega)}(\phi)$ occupying half of the corresponding $\phi$ interval.

## III. EXAMPLES

Consider the Ziff-Gulari-Barshad (ZGB) model [14], which reproduces the relevant features of carbon monoxide oxidation on a catalytic surface (a lattice whose sites can be either empty or occupied by an oxygen atom O or a carbon monoxide molecule CO). CO ($O_2$) reach the surface with probability $Y$ ($1-Y$). Whenever a CO encounters a vacant site, the site becomes occupied. If an $O_2$ molecule encounters two nearest-neighbor empty sites, it dissociates, filling the two sites. If two O atoms and one C atom reach an elementary $2\times 2$ lattice cell, they immediately form $CO_2$ and desorb. The model exhibits two transitions— regulated by the CO ($O_2$) molecule fraction $\rho_{\rm CO}$ ($\rho_{O_2}$)—each between an active steady state and an absorbing (poisoned) state. For large (extreme low) $Y$, the surface becomes saturated by CO (O). The former (latter) transition is discontinuous (continuous, belonging to the directed percolation, DP, universality class). The discontinuous transition is shown in Fig. 1. The $Y$ region

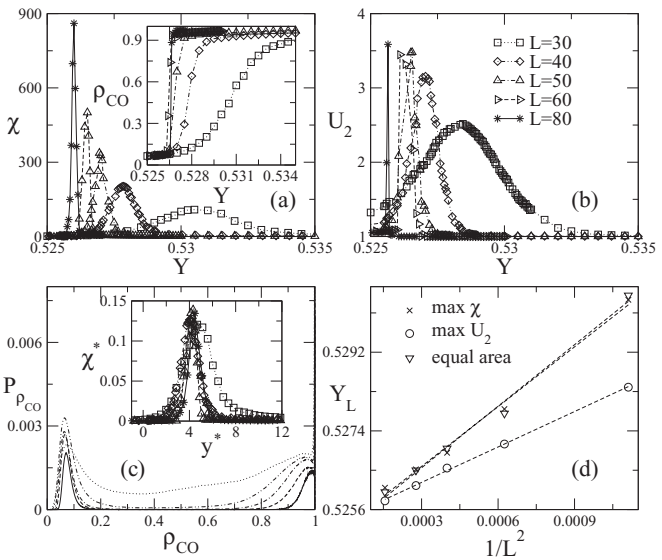


FIG. 1. The ZGB model. (a) The order parameter $\rho_{\rm CO}$ (inset) and its variance $\chi$ vs the creation probability $Y$. (b) The moment ratio $U_2$ vs $Y$. (c) The (non-normalized) order parameter QS probability distribution at the equal area condition. Inset: Data collapse analysis from the relations $\chi^* = \chi/L^2$ and $y^* = (Y - Y_0)L^2$. (d) Scaling of $Y_L$ as a function of $1/L^2$.

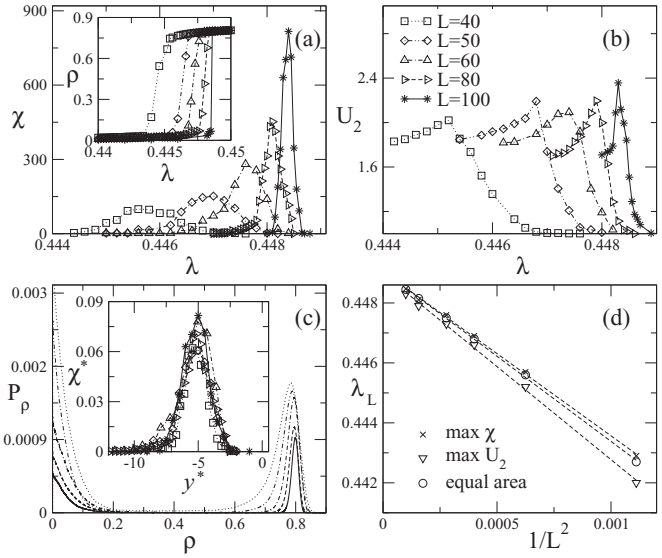


FIG. 2. The 2SCP model. (a) The order parameter $\rho$ (inset) and its variance $\chi$ vs the creation rate $\lambda$. (b) The moment ratio $U_2$ vs $\lambda$. (c) The (non-normalized) order parameter QS probability distribution at the equal area condition. Inset: Data collapse analysis from the relations $\chi^* = \chi/L^2$ and $y^* = (\lambda - \lambda_0)L^2$. (d) Scaling of $\lambda_L$ as a function of $1/L^2$.

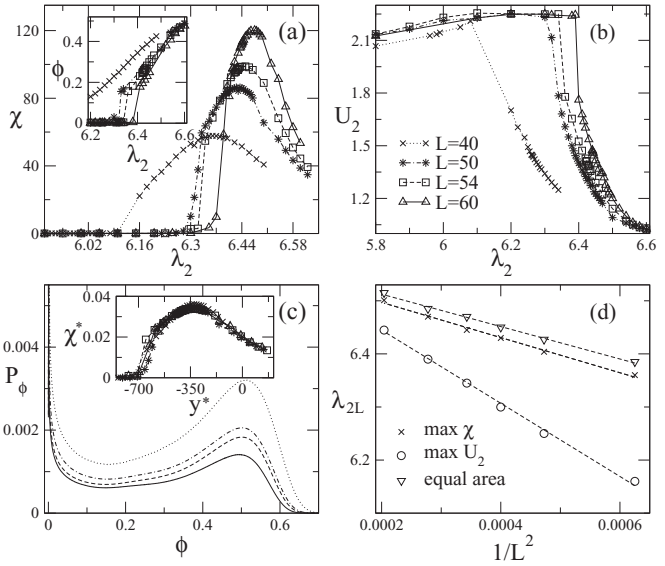


FIG. 3. The competitive CP ab-as transition. (a) The order parameter $\phi$ (inset) and its variance $\chi$ vs the creation rate $\lambda_2$. (a) The order parameter variance $\chi$ vs the creation rate $\lambda_2$. (b) The moment ratio $U_2$ vs $\lambda_2$. (c) The (non-normalized) order parameter QS probability distribution at the equal area condition. Inset: Data collapse analysis from the relations $\chi^* = \chi/L^2$ and $y^* = (\lambda_2 - \lambda_{20})L^2$. (d) Scaling of $\lambda_{2L}$ as a function of $1/L^2$.

of rapid increase of $\rho_{\rm CO}$ [inset of Fig. 1(a)] corresponds to the maxima of $\chi$ and $U_2$ [which increase with $L^2$, Figs. 1(a) and 1(b)] and their location scale with $1/L^2$ [Fig. 1(d)]. So, we estimate $Y_0 = 0.5253(3)$ (maximum of $\chi$) and $Y_0 = 0.5254(3)$ (maximum of $U_2$). The $Y_L$ for which the two peaks of $P_{\rho_{\rm CO}}$ [Fig. 1(c)] have the same area also scales with $1/L^2$. From this we estimate $Y_0 = 0.5253(3)$. These values are in excellent agreement among them and with $Y_0 = 0.5250(6)$, recently obtained by other means [36]. Defining $\chi^* = \chi/L^2$ and $y^* = (Y - Y_0)L^2$, the collapsed data are shown in the inset to Fig. 1(c), confirming a $L^2$ scaling.

For a two-species symbiotic contact process (2SCP) [16], any site is either empty or occupied by an element A, by an element B, or by one of each. Each element reproduces (autocatalytic), creating a new individual at one of its first-neighbor sites at a rate $\lambda_A = \lambda_B = \lambda$. In a single occupied site, A or B dies at a unitary rate. Sole individuals follow the usual CP dynamics [16]. However, in doubly occupied sites, due to symbiosis, both A and B die at a reduced $\mu = \text{const} < 1$ rate. Besides the usual CP active (A and B populations fixed) and absorbing phases, there are two extra symmetric active phases, in which just one species exists.

If A and B diffuse with rate $D$, for $\mu \to 0$ the transition changes from continuous to discontinuous. The order parameter is the density of occupied sites $\rho$. Figure 2 exemplifies this 2SCP for $\mu = 0.01$ and $D = 0.1$, with a discontinuous transition between absorbing and active symmetric phases for $\lambda \approx 0.449$ [16]. As ZGB, in the transition region there are peaks for $\chi$ and $U_2$ [Figs. 2(a) and 2(b)] whose maximum positions $\lambda_L$ increase with $1/L^2$ [Fig. 2(d)]. A $L \to \infty$ extrapolation yields $\lambda_0 = 0.4489(1)$ and $0.4490(1)$, respectively. The equal area condition for $P_\rho$ [Fig. 2(c)] shows a $1/L^2$ scaling, leading to $\lambda_0 = 0.4488(1)$. The estimates display excellent agreement among them and with Ref. [16]. Finally, a fair data collapse is shown in the inset to Fig. 2(c).

We discuss a model of competitive interactions in bipartite ($k = $ A and B) sublattices [48], assuming the version in Ref. [49], so instead of critical lines [48], the phase diagram has three coexistence lines. Also, besides an absorbing transition, we also have a spontaneous breaking symmetry transition. Given a site in the sublattice $k$, the number of particles in its first ($j = 1$) and second ($j = 2$) nearest neighborhood is $n_{jk}$. For $n_{jk}^{(a)}$, the number of adjacent particles in $j$, the dynamics is as follows [49]. With probability $[1 + \mu(n_{1k})^2]/[\lambda_1 + \lambda_2 + 1 + \mu(n_{1k})^2]$, we attempt to annihilate a randomly selected particle $P$. If $P$ survives, we choose at will $j = 1,2$. Then, with probability $p_j$ we try to create a new particle in a free site in the $j$ neighborhood of $P$, with $p_j = \lambda_j/[\lambda_1 + \lambda_2 + 1 + \mu(n_{1k})^2]$ for $n_{jk}^{(a)} \geqslant j$ and zero otherwise (in Ref. [48], $\mu = \lambda_2 = 0$).

The absorbing (ab)–active symmetric (as) phase line is discontinuous for lower $\lambda_1$. The proper order parameters are $\rho = (\rho_A + \rho_B)/2$ and $\phi = |\rho_A - \rho_B|$, with $\rho_X$ the $X$-sublattice density. In the ab phase we have $\rho = \phi = 0$, whereas for the as phase $\rho \neq 0$ and $\phi = 0$. So, for the as phase, the sublattices are equally populated. From Fig. 3 we see that the ab-as transition follows our FSS, yielding $\lambda_{20} = 6.571(5)$ (maximum of $\chi$), 6.58(1) (maximum of $U_2$) and 6.576(4) (equal areas).

Finally, we address two versions of the second Schlögl model [42]: SL1 [50,51], corresponding to a lattice version of the stochastic differential equation considered in Ref. [13], and SL2 [11], a modification of a pair contact process [52]. In SL$n$, a particle ($n = 1$) [a pair of two adjacent particles ($n = 2$)] is randomly selected and can be annihilated with

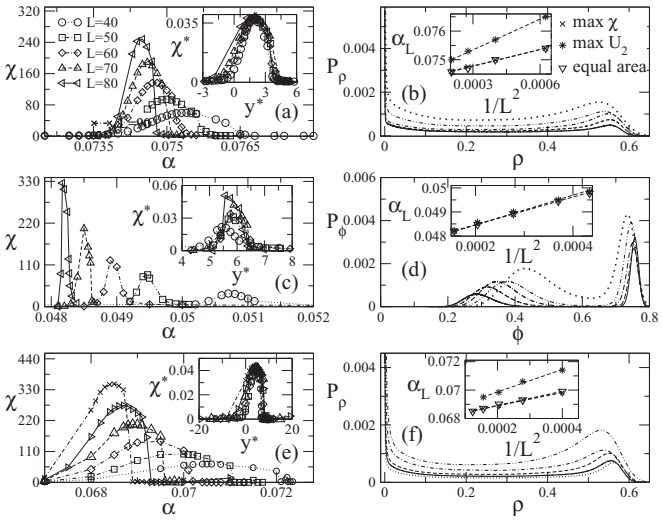


FIG. 4. The second Schlögl model: versions SL1 in (a) and (b), SL2 in (c) and (d), and SL1 with time disorder in (e) and (f). Left panels: The order parameter variance $\chi$ vs $\alpha$ (insets: their collapsed plots). Right panels: The (non-normalized) order parameter QS probability distributions (insets: $\alpha_L$ as a function of $1/L^2$).

probability $p_0 = \alpha/(1+\alpha)$. If it is not, then (1) for SL1, a nearest-neighbor site $i$ is chosen. If $i$ is empty, the particle diffuses to it. Otherwise, with probability $p = 0.5$ [50,51], a new particle is created and placed at will in a neighboring empty site. (2) If for SL2 there are at least $nn_p > 1$ other pairs in the original pair neighborhood, a new particle can be created with rate $nn_p/4$ in an available site in this same neighborhood.

SL1 (SL2) presents single (infinite) AS, with the order parameter being the particle density $\rho$ (pair density $\phi$). The transitions occur close to $\alpha = 0.0747$ (SL1) [51] and $\alpha = 0.0480$ (SL2) [11]. Results are summarized in Fig. 4. For both models our $\alpha_L$'s scale with $1/L^2$. For SL1, we obtain $\alpha_0 = 0.0742(1)$ (maximum of $\chi$), 0.0743(1) (maximum of $U_2$), and 0.0742(1) (equal areas). All estimates agree very well and are close to 0.0747 in Ref. [51] (calculated from the threshold separating the ongoing active state and an exponential decay of $\rho$, considering a fully occupied initial configuration). For SL2, $\alpha_0 = 0.0473(1)$ (maximum of $\chi$), 0.0472(1) (maximum of $U_2$), and 0.0472(1) (equal areas), all close to 0.0480 in Ref. [11] (derived from the onset for the decay of $\phi$ towards the absorbing regime).

Lastly, we incorporate temporal disorder into the SL1 model by assuming that at each instance, the creation probability $1 - p_0$ is $\min\{1/(1+\alpha)+\delta, 1\}$, with $\delta$ randomly chosen within $[-\sigma,\sigma]$. Results for $\sigma = 0.15$ are shown in Figs. 4(e) and 4(f). Here, also $\alpha_L$'s scales with $1/L^2$, from which we obtain $\alpha_0 = 0.0680(1)$ (maximum of $\chi$), 0.0683(2) (maximum of $U_2$), and 0.0680(1) (equal areas). Similar conclusions are obtained for $\sigma = 0.25$ (not shown), from which $\alpha_0 = 0.0265(1)$ (maximum of $\chi$ and equal areas). So, in contrast to spatial disorder [13], the present is an indication that temporal disorder does not hinder discontinuous absorbing phase transitions (but obviously further studies should be in order—see, e.g., Ref. [53]).

## IV. CONCLUSION

In summary, we propose a general FSS theory for discontinuous NEQPTs to AS. From QS ideas, we obtain an effective system—which reproduces the thermodynamic properties of the original problem—undergoing "normal" (i.e., not to AS) discontinuous phase transitions. Moreover, it is described by a bimodal distribution for the order parameter, therefore allowing inference to the $V$ scaling behavior. The only eventual difficulty in implementing such a universal scheme would be if the particular system hinders a QSPD. However, the known examples displaying such features are very specific [54]. Our study is particularly useful given that this class of NEQPTs have no equilibrium counterparts and universal treatments are lacking for discontinuous absorbing phase transitions for $d \geqslant 2$.

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