






Principal component analysis of absorbing state phase transitions

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We perform a principal component analysis (PCA) of two one-dimensional lattice models belonging to distinct nonequilibrium universality classes—directed bond percolation and branching and annihilating random walks with an even number of offspring. We find that the uncentered PCA of data sets storing various system's configurations can be successfully used to determine the critical properties of these nonequilibrium phase transitions. In particular, in both cases, we obtain good estimates of the critical point and the dynamical critical exponent of the models. For directed bond percolation, we are furthermore able to extract critical exponents associated with the correlation length and the order parameter. We discuss the relation of our analysis with low-rank approximations of data sets.

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I. INTRODUCTION

A significant milestone in theoretical physics has been the establishment of a classification of phase transitions in terms of universality classes at equilibrium, with field theory and renormalization group serving as major tools for understanding universality [1–4]. While phase transitions at thermodynamic equilibrium are relatively well understood, a complete understanding of out-of-equilibrium phase transitions is much less developed, although the techniques of renormalization group have also been extended to nonequilibrium dynamics [5,6]. Among the wide class of nonequilibrium, it is of particular interest to study those systems that are *intrinsically* out of equilibrium, i.e., that violate detailed balance. The main feature of these systems is the presence of probability currents between configurations [7]. Such systems include, for example, catalytic reactions and population dynamics, and they can be realized through nonequilibrium lattice models [8–10]. For these systems, no equilibrium counterpart is present.

A recent and promising avenue to enhance our comprehension of phase transitions involves the use of data-driven techniques, especially in their application to experimental contexts [11,12]. Notably, in recent years, both supervised and unsupervised machine learning techniques have demonstrated their capability to identify and characterize equilibrium phase transitions, even in systems featuring intricate nonlocal order parameters [13–20]. Whether the efficacy of these techniques extends to systems that are out of equilibrium remains relatively unexplored, although some investigations in this direction have been recently pursued [21–33].

The use of these methods not only presents intriguing challenges, but also raises profound questions. The essence of our understanding of phase transitions lies in fundamental concepts like coarse-graining and the renormalization group. These concepts have significantly influenced our grasp

of universality, revealing that few, coarse-grained variables suffice to decipher long-distance behavior. An intriguing question arises: can this understanding be extrapolated to the realm of data sets, and approached through the lenses of data science? Namely, is the intricacy of out-of-equilibrium many-particle dynamics also falling within the picture of dimensional reduction—not only in its capacity of describing critical properties using simple order parameters, but also at the level of governing the full state evolution? If so, to what extent? We note that linearized dimensional reductions have already been shown to be informative about information content in other many-body contexts, such as diagrammatic techniques [34].

In this study, we address these questions and investigate the applicability and effectiveness of unsupervised learning methods to identify nonequilibrium phase transitions, with a specific focus on absorbing phase transitions [35]. We conduct a principal component analysis (PCA) [36,37] study of two paradigmatic lattice models belonging to distinct nonequilibrium universality classes: the directed bond percolation (DBP) in the directed percolation (DP) universality class, and the branching and annihilating random walks with an even number of offspring (BARWe) in the parity-conserving (PC) universality class. Our study demonstrates that PCA can be successfully used to get information on data sets describing nonequilibrium phase transitions. Specifically, we accurately identify the critical point and dynamical critical exponent for both DP and PC universality classes. Furthermore, in the case of DP, we successfully extract critical exponents related to the correlation length and the order parameter. A significant implication of these findings is the efficacy of low-rank approximations in identifying universality classes within data sets.

The rest of this work is organized as follows. In Sec. II, we introduce the physical models considered in our study and the observables relevant to describe them. In Sec. III, we

describe the techniques and the data sets used in our analysis. In Sec. IV, we present the results of our analysis for DBP, while in Sec. V, we focus on the case of BARWe. Finally, in Sec. VI, we draw our conclusions and present possible outlooks.

II. MODELS

Lattice models play an important role in understanding equilibrium phase transition. The equilibrium properties of these models at inverse temperature β are determined by an energy function, the Hamiltonian H , which characterizes the equilibrium distribution $P_s(\mathcal{C}) \propto e^{-\beta H[\mathcal{C}]}$ of a configuration \mathcal{C} of the system. Nonequilibrium lattice models, instead, are defined by some dynamical evolution rules or, equivalently, by some set of transition probabilities $\{W(\mathcal{C} \rightarrow \mathcal{C}')\}$, which specify how the system evolves in time from configuration \mathcal{C} to \mathcal{C}' [10]. Unlike their equilibrium counterparts, the stationary probability distribution $P_s(\mathcal{C})$ of the configurations of these nonequilibrium lattice models is not known *a priori*. Indeed, $P_s(\mathcal{C})$ can only be determined as the solution of a master equation, which in most of the cases of statistical systems cannot be solved exactly.

In our study, we consider two lattice models defined in one spatial dimension which are driven out of equilibrium by the presence of an absorbing state, i.e., a state that cannot be left by the dynamics. The two models feature the same configuration space and have the same microscopic absorbing state, but they belong to different universality classes: directed bond percolation and branching and annihilating random walks with an even number of offspring. In both cases, the presence of an absorbing state implies that the system is out of equilibrium. Indeed, at equilibrium, the transition rates from one configuration to another should satisfy the condition of detailed balance $P_s(\mathcal{C})W(\mathcal{C} \rightarrow \mathcal{C}') = P_s(\mathcal{C}')W(\mathcal{C}' \rightarrow \mathcal{C})$ for every pair of configurations \mathcal{C} and \mathcal{C}' . In the case of an absorbing state \mathcal{C}_{abs} , the rate of leaving the absorbing configuration is $W(\mathcal{C}_{\text{abs}} \rightarrow \mathcal{C}') = 0$ for every \mathcal{C}' . For this reason, a system featuring an absorbing state cannot obey detailed balance,¹ making it a genuinely out-of-equilibrium system. In the following, we specify the dynamics of the two models under consideration.

A. Directed bond percolation

Directed percolation is the simplest and most common example of universality class exhibited by systems undergoing a transition from an active to an absorbing phase. Critical behavior associated with DP universality manifests in various systems, including, but not limited to, chemical reaction-diffusion models [38], the contact process [39], damage spreading transitions [40], surface growth with

¹We point out that the existence of an absorbing state \mathcal{C}_{abs} causes a violation of the detailed balance condition only if the stationary distribution $P_s(\mathcal{C})$ is not concentrated on \mathcal{C}_{abs} , i.e., if $P_s(\mathcal{C}) \neq \delta_{\mathcal{C}, \mathcal{C}_{\text{abs}}}$. This concentration actually occurs in systems of finite size, and thus a genuine nonequilibrium state may emerge only in the thermodynamic limit.

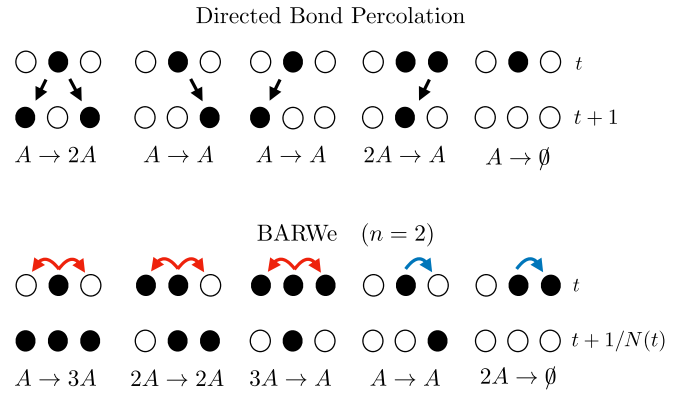


FIG. 1. Examples of moves for a three-site lattice for DBP and BARWe $n = 2$. For the BARWe, red arrows represent successful branching attempts, while blue arrows represent successful diffusion attempts. Notice that in the case of BARWe, the parity of the number of particles is conserved.

quenched disorder [41], Reggeon field theory [42,43], dissipative cold atoms [44], and measurement-induced phase transitions [45–48].

Being the most widespread universality class for nonequilibrium systems, we start our analysis with directed bond percolation, a nonequilibrium lattice model showing a transition in DP universality. We consider the evolution of DBP on a one-dimensional lattice of length L . The state of the system at discrete time t is specified by a configuration $\mathcal{C}_t = (x_{1,t}, \dots, x_{L,t})$, where each $x_{i,t}$ takes values 0 or 1 and indicates, respectively, an active or inactive site. Let the parameter $p \in [0, 1]$ be the percolation probability to the left and to the right. For a given configuration at time t , it is possible to determine the configuration at $t + 1$ according to the following evolution rule:

$$x_{i,t+1} = \begin{cases} 1 & \text{if } x_{i-1,t} = 1 \text{ and } z_i^- < p, \\ 1 & \text{if } x_{i+1,t} = 1 \text{ and } z_i^+ < p, \\ 0 & \text{otherwise,} \end{cases} \quad (1)$$

where z_i^{\pm} are i.i.d. random numbers uniformly distributed in $[0, 1]$.

Such dynamics can be interpreted as a reaction-diffusion process of a single-particle species A undergoing spontaneous decay $A \rightarrow \emptyset$, branching $A \rightarrow 2A$, and coagulation $2A \rightarrow A$, combined with single-particle diffusion. Examples of such processes are illustrated in Fig. 1. The “vacuum” state $\mathcal{C}_{\text{vac}} = (0_1, \dots, 0_L)$ is an absorbing state for the dynamics, since the spontaneous creation of particles (active sites) is not present.

B. Branching and annihilating random walks

Another well-established nonequilibrium universality class is the parity-conserving one, which was first observed in Refs. [49,50]. This universality class is the simplest possible deviation from the DP universality class and it emerges in various contexts, including branching and annihilating random walks [51], nonequilibrium Ising models [52], systems with two absorbing states [53,54], roughening transitions [55], and entanglement dynamics [56,57].

Among the models that belong to the PC universality class, we shall focus here on a special case of the branching and annihilating random walks (BARWs). The latter are models of particles on a lattice that can diffuse, produce offspring on neighboring sites, and annihilate upon contact. If interpreted as a reaction-diffusion process, this dynamics involves a single species of diffusing particles that may produce n offsprings $A \rightarrow (n+1)A$ or annihilate in pairs $2A \rightarrow \emptyset$ [51]. For even n , this kind of dynamics conserves the number of particles modulo 2, and thus given an initial state with an even (odd) particle number, the dynamics remains confined in the even (odd) parity sector. When the dynamics starts from a state with an even number of particles, the vacuum state is a reachable absorbing state for the dynamics.

Here we consider the microscopic model formulated in Ref. [58], corresponding to $n = 2$, i.e., a special case of the branching and annihilating random walk with an even number of offsprings (BARWe). In this model, like in the previous one, the state of the system at time t is specified by a configuration $\mathcal{C}_t = (x_{1,t}, \dots, x_{L,t})$. The update rule for the configuration is formulated as follows: A particle at site i is randomly chosen. This particle makes an offspring production attempt on the two neighboring sites with probability p or a diffusion attempt to a randomly chosen neighboring site with probability $1 - p$. Whenever the neighboring sites involved in the attempted offspring production or diffusion are occupied, the move is accepted with probability k_a , and annihilation of the neighboring particles with the offspring occurs, while with probability $1 - k_a$ the move is rejected. If instead the attempted move involves only unoccupied neighboring sites, the move is always accepted. Each time a particle is selected, a time counter is increased by $1/N(t)$, where $N(t)$ is the number of particles at time t , such that in a time step each particle either branches or diffuses a single time, on average. In our analysis, we fix the annihilation rate to be $k_a = \frac{1}{2}$.

C. Observables and phase transitions

For both models, a pivotal quantity is the average density of active sites,

$$\rho(t) = \left\langle \frac{1}{L} \sum_{i=1}^L x_{i,t} \right\rangle, \quad (2)$$

where $\langle \dots \rangle$ denotes an average over an ensemble of realizations of the stochastic evolution. In the limit of infinite system size $L \rightarrow \infty$ and as p is increased, both models undergo a continuous transition from the absorbing phase to the active phase. In the case of the BARW, this also requires having an even initial number of particles. This transition, occurring at a model-dependent value p_c of p , can be detected by the stationary density of active sites

$$\rho_\infty = \lim_{t \rightarrow \infty} \rho(t) \quad (3)$$

as an order parameter that is zero in the absorbing phase, while it attains a nonzero value in the active phase. For values of p close to the critical point p_c , the stationary density behaves as

$$\rho_\infty \sim (p - p_c)^\beta \quad (p > p_c). \quad (4)$$

TABLE I. Estimates of the values of the critical points p_c for the directed bond percolation (DBP) and for the BARWe with $n = 2$ [58] and of the universal critical exponents for the corresponding universality classes, i.e., respectively, directed percolation (DP) [8,59,60] and parity-conserving (PC) (the estimates for β , ν_\perp , ν_\parallel were obtained from the $n = 4$ BARW in Ref. [61], while the estimates for z and α are taken from [62] for the $n = 2$ BARW), in one spatial dimension. In $d = 1$ both DP and PC have $\alpha = \delta$, where δ is the exponent characterizing the decay of the survival probability [9].

Quantity	DBP ($d = 1$) [8,59]	BARW $n = 2$ ($d = 1$) [58]
p_c	0.6447001(1)	0.4946(2)
	DP ($d = 1$) [8,60]	PC ($d = 1$) [61–63]
β	0.276486(8)	0.92(3)
ν_\perp	1.096854(4)	1.84(6)
ν_\parallel	1.733847(6)	3.25(10)
z	1.580745(10)	1.7415(5)
α	0.159464(6)	0.2872(1)

When the dynamics starts from a fully active configuration, at the critical point $p = p_c$, the density of particles shows an algebraic decay

$$\rho(t) \sim t^{-\alpha}. \quad (5)$$

In addition, it is possible to define correlation functions [64]:

$$C(|i - j|) = \lim_{t \rightarrow \infty} \left\langle \frac{1}{t} \sum_{\tau=0}^t (x_{i,\tau} - \bar{x})(x_{j,\tau} - \bar{x}) \right\rangle, \quad (6)$$

$$C(t) = \lim_{L \rightarrow \infty} \left\langle \frac{1}{L} \sum_{i=1}^L (x_{i,0} - \bar{x})(x_{i,t} - \bar{x}) \right\rangle, \quad (7)$$

where we introduced $\bar{x} = \lim_{t \rightarrow \infty} \frac{1}{t} \sum_{\tau=0}^t \langle x_{i,\tau} \rangle$, which actually does not depend on the site index i . Far from criticality, these correlation functions decay exponentially as

$$C(|i - j|) \sim e^{-|i-j|/\xi_\perp}, \quad (8)$$

$$C(t) \sim e^{-t/\xi_\parallel}, \quad (9)$$

and their exponential decay defines the correlation length ξ_\perp and the correlation time ξ_\parallel . Close to criticality $p \rightarrow p_c$, these quantities diverge as

$$\xi_\perp \sim |p - p_c|^{-\nu_\perp}, \quad (10)$$

$$\xi_\parallel \sim |p - p_c|^{-\nu_\parallel}. \quad (11)$$

The anisotropy between the time and space directions is quantified by the dynamical critical exponent $z = \nu_\parallel/\nu_\perp$, which relates the divergence of the correlation time ξ_\parallel to that of the correlation length ξ_\perp as $\xi_\parallel \sim \xi_\perp^z$.

The transition from the absorbing to the active phase is known to belong to the DP universality class for DBP and to the PC universality class for the BARWe (investigated for $k_a = 1/2$ in Ref. [58]). The critical points of both models in one spatial dimension $d = 1$, together with the corresponding universal exponents of the DP and PC universality classes, are reported in Table I.

In a numerical simulation, however, the system size L is finite. This implies that there is always a finite probability

of ending in the absorbing state $\mathcal{C}_{\text{vac}} = (0_1, \dots, 0_L)$ and thus, in the infinite-time limit, the system always reaches it, i.e., $\rho_\infty = 0$. Although a *bona fide* active stationary state exists only for $L \rightarrow \infty$, finite-size systems, in the active phase, display a quasistationary behavior: after a transient, physical quantities do not change significantly for some time, before attaining the values corresponding to the absorbing state. Upon increasing L , the duration of this quasistationary behavior rapidly increases and the observables converge to their stationary values. Close to criticality, the quasistationary state is reached from a generic initial condition in a timescale $t_c \sim L^z$. Accordingly, in order to study the active state from simulations of finite systems, we focus on this quasistationary state by considering the observables at times $t \simeq t_c$.

III. METHODS AND DATA SETS

A. Principal component analysis

Principal component analysis can be regarded as an application of the singular value decomposition (SVD) [65] as a compression algorithm. Let us consider N_r realizations (or observations) of a vector of m variables $\vec{x}^{(\mu)} = (x_1^{(\mu)}, \dots, x_m^{(\mu)}) \in \mathbb{R}^m$, with $\mu = 1, \dots, N_r$. Each observation is a data point in \mathbb{R}^m . In the case of a physical system, one can think of m as the number of degrees of freedom that describe the state of the system. Given the ensemble of observations $\{\vec{x}^{(\mu)}\}_{\mu=1}^{N_r}$, we can introduce an $N_r \times m$ data matrix

$$\mathbf{X} = (\vec{x}^{(1)}, \dots, \vec{x}^{(N_r)})^T, \quad (12)$$

having the observations as rows. We introduce $\tilde{\mathbf{X}}$, the *centered data matrix*, as the matrix having components

$$\tilde{\mathbf{X}}_{\mu i} = \mathbf{X}_{\mu i} - \frac{1}{N_r} \sum_{\mu'=1}^{N_r} \mathbf{X}_{\mu' i}. \quad (13)$$

$\tilde{\mathbf{X}}$ is characterized by the fact that, contrary to \mathbf{X} , the arithmetic average of its rows vanishes. Starting from \mathbf{X} and $\tilde{\mathbf{X}}$, one can construct two $m \times m$ matrices that encode information about correlations present in the data set: the *empirical covariance matrix*

$$\mathbf{\Sigma} = \frac{1}{N_r} \tilde{\mathbf{X}}^T \tilde{\mathbf{X}}, \quad (14)$$

and the *empirical second-moment matrix*

$$\mathbf{M} = \frac{1}{N_r} \mathbf{X}^T \mathbf{X}. \quad (15)$$

For the sake of brevity, we will refer to $\mathbf{\Sigma}$ and \mathbf{M} simply as covariance and second-moment matrices. We denote the spectra of $\mathbf{\Sigma}$ and \mathbf{M} as $\{\lambda_i^c\}$ and $\{\lambda_i^u\}$, respectively, with $i = 1, \dots, m$, where the eigenvalues are sorted in nonincreasing order, i.e., $\lambda_i^{c/u} \geq \lambda_{i+1}^{c/u}$. Let us notice that the number of nonzero eigenvalues of $\mathbf{\Sigma}$ or \mathbf{M} is upper-bounded by their rank. This rank is the same as the corresponding data matrix and thus it is smaller than or equal to $\min(N_r, m)$. The procedure of computing eigenvalues and eigenvectors of either the second moment or the covariance matrix is directly related to computing the SVD decomposition of \mathbf{X} or $\tilde{\mathbf{X}}$, with the eigenvalues being related to the singular values σ_i of the

corresponding matrices as $\lambda_i^u = \sigma_i^2(\mathbf{X})/N_r$ or $\lambda_i^c = \sigma_i^2(\tilde{\mathbf{X}})/N_r$, respectively, and the eigenvectors being the right singular vectors of the corresponding data matrix.

1. PCA spectrum

Some of the quantities of primary interest in PCA are the normalized eigenvalues $\pi_i^{c/u}$ of the aforementioned matrices, i.e.,

$$\pi_i^{c/u} = \frac{\lambda_i^{c/u}}{\sum_{i=1}^{\min(N_r, m)} \lambda_i^{c/u}}. \quad (16)$$

Since both the covariance matrix and the second-moment matrix are positive-semidefinite, the quantities $\{\pi_i^{c/u}\}$ can be formally regarded as probability distributions, as they satisfy the properties of being normalized and non-negative. In the case of the centered data $\tilde{\mathbf{X}}$, the quantities π_i^c represent the percentage of variance along the i th principal eigenvector of the covariance matrix $\mathbf{\Sigma}$, and for this reason $\{\pi_i^c\}$ is referred to as the *explained variance ratio*. A small explained variance along one eigendirection implies that the data are not much spread along that direction, and they can thus be regarded as lying on a lower-dimensional space.

2. PCA entropies

The use of PCA as a compression algorithm involves a selection of $k < m$ eigenvectors associated with the k largest normalized eigenvalues onto which the data set is then projected. In many physical cases, however, there is no sharp separation between the magnitude of the various components, and the truncation cutoff is arbitrarily chosen case by case. A possible way to account for the full PCA spectrum is to introduce information-theoretic quantities such as entropies [66–68]. Given the normalized spectrum $\{\pi_i^{c/u}\}$ one can define Renyi-PCA entropies of order n as

$$S_{\text{PCA},n}^{c/u} = \frac{1}{1-n} \log \left(\sum_i (\pi_i^{c/u})^n \right), \quad (17)$$

which we call *Renyi-PCA entropies*. All the Renyi-PCA entropies satisfy

$$S_{\text{PCA},n}^{c/u} \leq \log(\min(N_r, m)), \quad (18)$$

as they attain their maximum value on the uniform distribution. We refer to the particular case $n \rightarrow 1$ as PCA-entropy,

$$S_{\text{PCA}}^{c/u} = - \sum_i \pi_i^{c/u} \log \pi_i^{c/u}. \quad (19)$$

These quantities provide information about the compressibility of the data, as they can serve as a measure of the flatness of the PCA spectrum. For example, if the explained variance ratio is uniform, one expects that all the components are relevant to describe the data set, and thus the data set cannot be compressed and visualized in terms of a lower-dimensional space. Moreover, it has recently been shown that these quantities can be used to extract critical behavior both in equilibrium classical systems and disordered quantum systems [69,70].

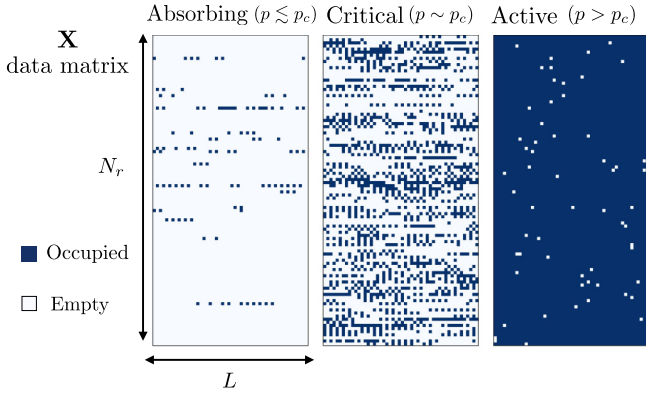


FIG. 2. Examples of data matrices \mathbf{X} constructed from $N_r = 100$ spatial configurations $\bar{x}^{(\mu)}$ of directed percolation on a lattice with $m = L = 50$, extracted at time t_c from independent Monte Carlo simulations. These examples refer to three different values of p which, from left to right, correspond to the absorbing, critical, and active phases for $L \rightarrow \infty$.

B. Data sets

In our analysis, we examine both Σ and \mathbf{M} in the quasistationary state and as a function of time. Concerning the study of quasistationarity, with *steady-state dataset* we refer to the collection of data matrices storing configurations $\{\bar{x}^{(\mu)}\}_{\mu=1}^{N_r}$ taken at time $t_c = L^z$ and extracted from independent simulations. In this case, one has to analyze a set of data matrices that store configurations for a given p and L . With *time-dependent dataset*, instead, we refer to the collection of data matrices for different times. In this case, data matrices for different p , L , and t are analyzed. In all our analyses, the data matrices \mathbf{X} and $\tilde{\mathbf{X}}$ have dimensions $N_r \times L$ and store the configurations of the specific model under study, obtained by evolving it from an initial active state $\mathcal{C}_{\text{full}} = (1_1, \dots, 1_L)$ in which all lattice sites are occupied. Examples of such data matrices are shown in Fig. 2. The observations $\bar{x}^{(\mu)}$ have dimension $m = L$ and each of them denotes a point on an L -dimensional unit hypercube. For all of our simulation data, we choose $N_r > L$, which allows us to estimate second-moment matrix elements in a statistically accurate way [71]. Choosing $N_r < L$ would not be statistically significant, as it is not possible to reconstruct faithfully L^2 correlations using $O(LN_r) < L^2$ data.

To provide a data-driven characterization of the samples, two approaches are possible. If one is interested in studying fluctuations of the data with respect to its mean, then centering the data is the appropriate choice [72]. Most applications of PCA indeed involve a centering of the data $\mathbf{X} \mapsto \tilde{\mathbf{X}}$ [see Eq. (13)], followed by the analysis of the covariance matrix Σ , which is directly obtained from $\tilde{\mathbf{X}}$. Connections between the properties of PCA of centered and uncentered matrices are discussed in Ref. [73].

In the present case, instead, we find that the data analysis obtained without centering the data is more suited to making qualitative and quantitative statements. As noted in the literature [37], this type of analysis can be relevant if the data are such that the origin is an important point of reference. This is in fact the case in our study, since the origin, for both models under study, represents their absorbing state

configuration, namely $\mathcal{C}_{\text{vac}} = (0_1, \dots, 0_L)$. Hence, here it is physically meaningful to study the variation of the data about this point. In fact, the emergence of a finite spatial density of particles in the system corresponds to an average displacement of the data points from the origin. Accordingly, the center of mass of the data \mathbf{X} contains important information about the phase in which the system is. In our specific case, the data points $\bar{x}^{(\mu)}$ lie on the vertices of an L -dimensional unit hypercube, given that $x_i^{(\mu)} \in \{0, 1\}$ with $i = 1, \dots, L$. As the probability p is increased (see Sec. II), one expects the data to move from being close to the origin—which corresponds to the absorbing state—to being displaced towards the corner that is the farthest from it—corresponding to the fully occupied active state. The displacement of the centroid of the data from the origin is therefore related to the presence of an active phase.

A natural question that arises is whether the spectral properties of the covariance matrix Σ or of the second-moment matrix \mathbf{M} , which are naturally expected to be sensitive to such a change, can be used to characterize the kind of transition undergone by the system as p is varied. In our examination below, we find that both kinds of analyses can be used to describe the presence of such a phase transition, with an explicit connection to physical observables in the uncentered case. In view of this connection, below we focus on the analysis of \mathbf{M} , while we present the results concerning Σ in Appendix A. Let us note, in addition, that also a centered analysis based on the quantified principal components, defined and discussed in Appendix B for DBP, can be physically informative.

IV. RESULTS FOR DIRECTED BOND PERCOLATION

A. Largest normalized eigenvalue

When characterizing a phase transition, the first step is to determine the critical point. In the case of directed percolation, the critical value p_c of the probability p can be determined by looking at the temporal evolution of the particle density $\rho(t)$, starting from a fully active configuration. In fact, at the critical point $p = p_c$, $\rho(t)$ is expected to decay algebraically to zero as in Eq. (5). In the absorbing regime, instead, an exponential decay, $\rho(t) \sim e^{-t/\xi_{||}}$, is expected, while in the active phase $\rho(t)$ approaches a nonvanishing quasistationary plateau value [10].

In Fig. 3, we verify whether a similar behavior holds for the largest normalized eigenvalue π_1^u . In particular, we show three curves for $\pi_1^u(t)$ obtained for values of p close to p_c . We find that the critical point p_c can be approximately determined by checking when the longest-lived algebraic decay occurs ($p = 0.64$). In addition, the decay exponent for $\pi_1^u(t)$ at the critical point is in reasonable agreement, considering the modest system size and the value of p , with the exponent α which controls the decay of the density (and which was determined via accurate Monte Carlo simulations; see Table I). We emphasize that this basic factual observation is actually the starting point for the more refined analysis we present below. This is a first clear indication that the PCA spectrum already carries considerable information about the system.

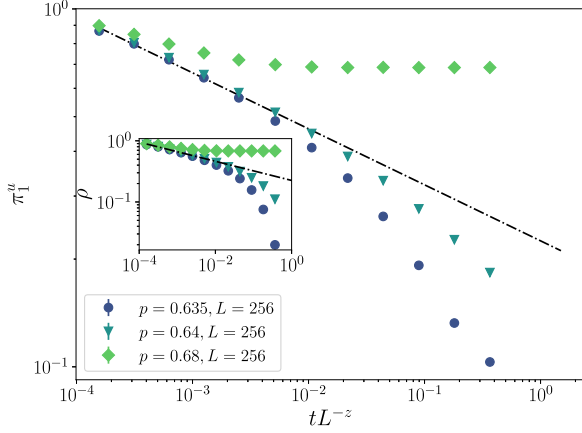


FIG. 3. Largest normalized eigenvalue π_1^u for DBP, as a function of time, obtained from the uncentered PCA analysis with $N_r = 3000$ and for various values of p . Points are averaged over five repetitions. The standard deviation of the points is smaller than the size of the markers. The inset shows the corresponding density ρ of active particles. The dotted-dashed line is a guide to the eye and corresponds to $\alpha = 0.157$ [see Eq. (5)].

We then examine if and how the steady-state values of the largest normalized eigenvalue π_1^u and the particle density ρ are related by plotting their ratio ρ/π_1^u as a function of p , shown in Fig. 4 for various values of the system size L . Upon increasing L , the ratio appears to converge to $\simeq 1$ in the active phase, while we find that it decreases near the critical point and it keeps doing so upon decreasing p within the absorbing phase.

Panel (a) of Fig. 5 shows the dependence of the stationary value of π_1^u on the probability p close to the transition point (vertical dash-dotted line) for various values of the system size L . Upon increasing L , the value of π_1^u shows a clear inflection close to p_c , as one would expect for the order parameter of a continuous phase transition. For the largest value of L considered in panel (a), Fig. 5(b) shows the dependence on p of the largest four eigenvalues $\pi_{1,2,3,4}^u$ and of π_8^u close to the transition point. This shows that, in the active phase, the largest

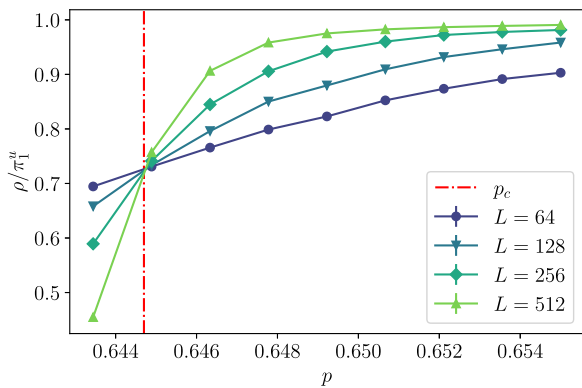


FIG. 4. Behavior of the ratio ρ/π_1^u for DBP. While above the critical point the two quantities show extremely good agreement, below the critical point the first uncentered normalized eigenvalue has a smaller overlap with the density. Each point is obtained using $N_r = 2000$ and averaging over five repetitions.

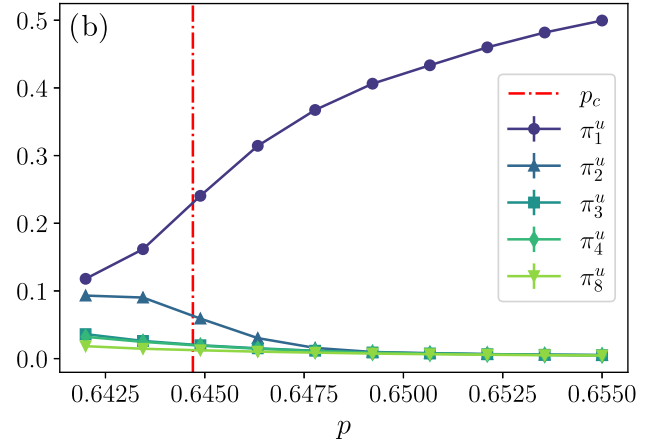
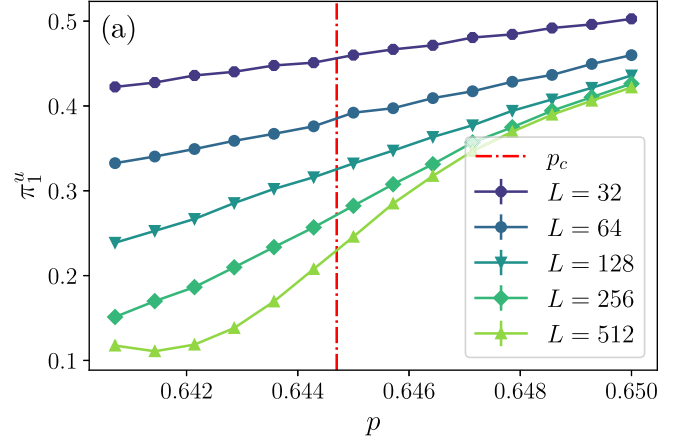


FIG. 5. (a) Largest uncentered normalized eigenvalue π_1^u in the vicinity of the critical point obtained for $N_r = 3000$. Each data point is averaged over five realizations. (b) Behavior of the first few largest normalized eigenvalues for DBP close to the critical point for $L = 512$, $N_r = 2000$. Each point is averaged over five repetitions. Upon increasing the probability p towards the active phase, most weight of the normalized spectrum is contained in the first principal component. At the critical point $p = p_c$, the system still shows a clear separation of magnitude between the first component, i.e., the largest eigenvalue, and the others.

eigenvalue is actually significantly larger than the others, such that the ratio ρ/π_1^u tends to 1 in the active phase. As we show below, π_1^u can be used to extract some universal features of the transition. In particular, we perform a finite-size scaling analysis of π_1^u obtained from a PCA based on the steady-state configurations of DBP. We assume the finite-size scaling form

$$\pi_1^u(p, L) = L^\omega f((p - p_c)L^\zeta). \quad (20)$$

If the direct relationship between π_1^u and the particle density ρ holds, the values of the exponents ω and ζ are expected to match those which result in a corresponding scaling collapse of the density ρ . These exponents are given by $\omega = -\beta/\nu_\perp \approx -0.252$ and $\zeta = 1/\nu_\perp \approx 0.911$. To perform the finite-size scaling analysis, we adopt the method of Ref. [74], which is described in Appendix C. We denote by p_* , ω_* , and ζ_* the values of p_c , ω , and ζ which lead to the best data collapse on a master curve f .

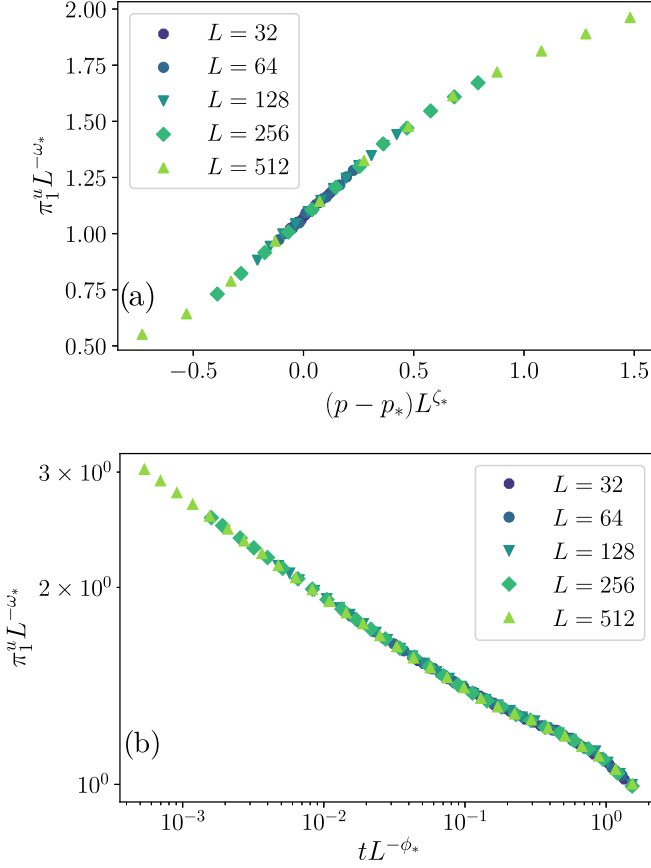


FIG. 6. (a) Finite-size scaling of π_1^u in the steady state. The values for which the best data collapse is obtained are $p_* = 0.644\,74(5)$, $\zeta_* = 0.904(4)$, $\omega_* = -0.246(3)$. (b) Time-dependent finite-size scaling of π_1^u . The estimated values are $\phi_* = 1.58(2)$, $\omega_* = -0.248(3)$. In both cases, data were obtained for $N_r = 3000$ and each data point is a result of an average over five realizations.

In Fig. 6, we report the finite-size scaling analysis performed on the basis of the lattice configurations in the steady state, finding good agreement of $\omega_* = -0.246(3)$ and $\zeta_* = 0.904(4)$ with the values ω and ζ of the DP universality class reported above. This fact indicates that, although π_1^u is not the particle density, it captures the critical properties in a similar manner. A way to extract further information on the critical exponents is to perform a finite-size scaling of the time dependence of π_1^u for $p = p_c$, i.e., during its relaxation towards the vanishing stationary value. In this case, we use the scaling form

$$\pi_1^u(L, t) = L^\omega g(tL^{-\phi}), \quad (21)$$

where, still assuming that π_1^u behaves as the particle density, ω is given as discussed after Eq. (20) and $\phi = z = 1.580$ in terms of the exponents in Table I. Figure 6 shows the result of the finite-size scaling. Also in this case, values $\omega_* = -0.248(3)$ and $\phi_* = 1.58(2)$ determined from the best data collapse are fairly close to the values expected for the DP universality class.

B. Analytical relation between principal components and order parameter

The similarity in the scaling properties of the largest normalized eigenvalue π_1^u and of the density ρ , illustrated in Fig. 4, can be understood through considerations on the SVD of the data matrix \mathbf{X} . Given an $n \times n'$ matrix A , we can perform its SVD decomposition and write $A = UDV^T$, where D is an $r \times r$ diagonal matrix, with $r = \text{rank}(A)$, having the singular values $\sigma_i(A)$ ($i = 1, \dots, r$) along the diagonal, while U and V^T store the singular vectors \mathbf{u}_i and \mathbf{v}_i^T , respectively, of A . In terms of these singular vectors, the SVD decomposition of A can be written as

$$A = \sum_{i=1}^r \sigma_i(A) \mathbf{u}_i \mathbf{v}_i^T. \quad (22)$$

We can define the truncation A_k of A to the first k largest singular values (with $k < r$) as

$$A_k = \sum_{i=1}^k \sigma_i(A) \mathbf{u}_i \mathbf{v}_i^T, \quad (23)$$

where the matrix A_k has rank k . It is possible to show that this decomposition is optimal among all the possible rank- k approximations [72,75]. This means that, for any matrix B of rank at most k , the following inequality holds:

$$\|A - A_k\|_F \leq \|A - B\|_F, \quad (24)$$

where the Frobenius norm $\|\cdot\|_F$ of a matrix A is defined as $\|A\|_F = \sum_{ij} A_{ij}^2$. Accordingly, the error made by approximating A with A_k is smaller than the error that one would make by approximating it with any other matrix of rank at most k . In this respect, A_k is said to be the best rank- k approximation of A . Note that the sum of the squared singular values $\sigma_i^2(A)$ of a matrix A equals the Frobenius norm $\|A\|_F$ of the matrix [72] (see, e.g., Ref. [65] for a proof). For a binary data set $X_{\mu i} = x_i^{(\mu)} \in \{0, 1\}$, such as the one considered in the present work, one has $X_{\mu i}^2 = X_{\mu i}$ and thus

$$\|\mathbf{X}\|_F = \sum_{\mu=1}^{N_r} \sum_{i=1}^L X_{\mu i}^2 = \sum_{\mu=1}^{N_r} \sum_{i=1}^L X_{\mu i} = N_r L \rho, \quad (25)$$

where in the last equality we used the definition of the density. This equality implies that

$$\sum_{i=1}^r \sigma_i^2(\mathbf{X}) = N_r L \rho, \quad (26)$$

or, equivalently,

$$\sum_{i=1}^r \lambda_i^u = L \rho, \quad (27)$$

where λ_i^u are the unnormalized eigenvalues of the second moment matrix \mathbf{M} , which are related to σ_i^2 as discussed after Eq. (15).

Equation (27) expresses the equality of the trace of \mathbf{M} in the original basis and in the basis that diagonalizes \mathbf{M} . When a clear difference in the order of magnitude emerges between the first (largest) eigenvalue and the remaining ones, one can neglect the subleading contributions given by the

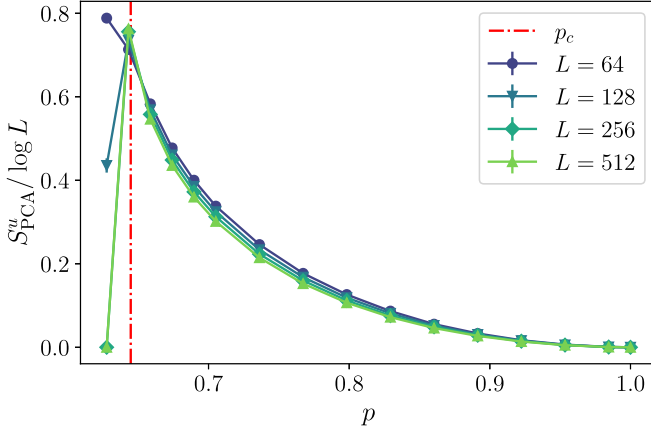


FIG. 7. Normalized uncentered PCA entropy. As the system size L increases, the entropy shows a transition in the vicinity of the critical point. Data points are obtained using $N_r = 2000$. Each data point is the result of an average over five repetitions.

latter to Eq. (27), finding that $\lambda_1^u/L \simeq \rho$. This is precisely what is observed deep within the active phase where, as p increases, the rank of \mathbf{X} tends to be 1, and most of the weight tends to be contained in the first principal component. Although Eq. (27) involves the largest unnormalized component λ_1^u , our numerical results show that also π_1^u and ρ are related. In particular, deep in the active phase where $\lambda_1^u \gg \lambda_{i>1}^u$, π_1^u and ρ have the strong overlap displayed in Fig. 4, while at the critical point, the relationship between these two quantities is weakened by the fact that part of the spectral weight is due to other components. Nevertheless, also close to the critical point, the largest uncentered explained variance π_1^u shows a scaling behavior compatible with that of the density. Keeping only the truncation of \mathbf{X} to the largest uncentered component is what is called the *best rank-1* truncation. Accordingly, the numerical data and analytic arguments presented above suggest that the best rank-1 truncation of the data is already able to capture and reproduce the critical behavior of DBP.

C. PCA entropies

Entropies can also play a role in the characterization of absorbing state phase transitions [76,77]. It is natural to wonder whether information-theoretic quantities, such as the Renyi-PCA entropies defined in Sec. III, which involve the entire PCA spectrum beyond the largest eigenvalues considered above, can be sensitive to critical behavior.

In Fig. 7, we show the steady-state uncentered PCA entropy defined in Eq. (19) as a function of p , for system sizes $L \in [64, 512]$, normalized to the maximum value it can attain ($\log L$). This quantity displays a peak in the vicinity of the critical point, marked by the vertical dash-dotted line. In the limit of infinite system size, no points are expected for $p < p_c$, as no fluctuations occur in the absorbing phase, and the PCA entropy should be exactly zero. The same kind of behavior is also seen in all the Renyi entropies in Eq. (17), as discussed in Appendix D.

To better understand the nature of the PCA entropy, we want to compare it with other commonly used measures of information in statistical mechanics. The most suitable

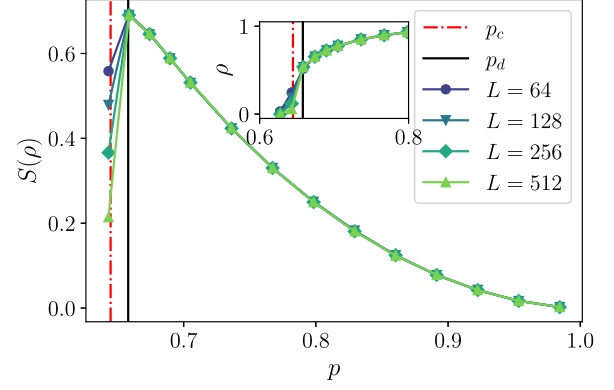


FIG. 8. Shannon entropy of the order parameter, obtained for $N_r = 2000$. Each data point is the result of an average over five repetitions. The inset shows the density ρ of the active particles as a function of p . The peak of the Shannon entropy corresponds to the value p_d of p , where the density attains the value $1/2$.

comparison would be the one with the Shannon entropy $S(\mathbf{X})$ of the data set, which is inaccessible, as the entries of \mathbf{X} are correlated and the probability distribution of \mathbf{X} is unknown at any time, even in the stationary state. We note that, under specific circumstances, PCA and Shannon entropies may be closely related [70], although here it is not the case. To have another candidate, we compare the PCA entropy with the Shannon entropy of the order parameter ρ , namely,

$$S(\rho) = -\rho \log \rho - (1 - \rho) \log(1 - \rho). \quad (28)$$

The reason to consider this quantity is that, within a mean-field approximation, treating the variables $x_i^{(\mu)}$ as uncorrelated, with $x_i^{(\mu)} = 1$ with probability $\rho(p)$ and $x_i^{(\mu)} = 0$ with probability $1 - \rho(p)$, one would naturally assign to the uncentered data set \mathbf{X} an entropy $S(\mathbf{X}) = N_r L S(\rho)$. In the present case, it turns out that the Shannon entropy displays a peak at a value $p_d \approx 0.658 > p_c$ of the probability p , as shown in Fig. 8. Correspondingly, the density ρ takes the value $\rho = 1/2$. Comparing the behavior of the PCA and the Shannon entropy, we conclude that the former features a strong non-mean-field character.

V. RESULTS FOR BRANCHING AND ANNIHILATING RANDOM WALKS

In this section, we apply the analysis previously performed for directed bond percolation to the case of branching annihilating random walks with an even number of offspring, which display an absorbing phase transition belonging to the PC universality class. For parity-conserving models, however, particular care has to be used when analyzing the data sets. In fact, as pointed out in Ref. [61], quasistationarity of observables is better observed by performing averages that take into account only the configurations that are not in the absorbing state. For this reason, after having computed the data matrices by storing the N_r realizations of the dynamics of the model, we discard the configurations that have reached the absorbing state. All the analysis we present in this section is thus based exclusively on these surviving configurations, which means that the PCA is performed on matrices where inactive

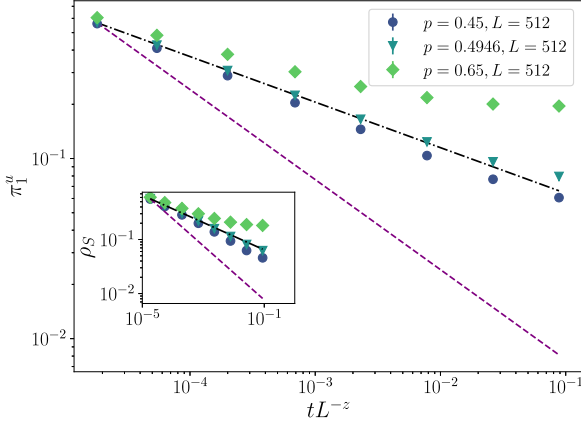


FIG. 9. Largest normalized eigenvalue π_1^u as a function of time, obtained from uncentered PCA analysis with $N_r = 3000$ for BARW. Points are averaged over five repetitions. The inset shows the corresponding density. The dotted-dashed line is obtained from a fit and corresponds to $\alpha = 0.253$, which deviates from the expected value 0.285(2) reported in Table I. The dashed line, instead, reports the expected decay for $p < p_c$, associated with $\alpha = 1/2$.

configurations are removed, and only active configurations are taken into account. To distinguish the density computed over surviving samples from that defined in Eq. (2), we denote the former as ρ_S . To simplify the notation, hereafter we do not add the subscript S to the other quantities, but we understand that they are computed over the surviving samples.

A. Largest normalized eigenvalue

As we did for DBP, we first analyze the behavior of the largest normalized uncentered eigenvalue π_1^u as a function of time, which is reported in Fig. 9 for three values of p corresponding to the active, critical, and absorbing phase and with $L = 512$. In this case, the analysis is complicated by the fact that in parity-conserving models the decay of the density $\rho(t)$ as a function of time t is algebraic also within the absorbing phase [8]. Indeed, such algebraic decay is observed in Fig. 9 both for π_1^u and ρ_S . The expected power-law decay in the absorbing phase is the one associated with the pair-annihilation fixed point in one dimension $\alpha = 1/2$ (see Refs. [78,79]), and it is shown in Fig. 9 as a dashed line. As a matter of fact, this power can be observed in numerical simulations only at very low values of p or at very large system sizes, and the decay exponent varies continuously for finite system sizes. For the sizes accessible to our numerical simulations (up to $L = 512$), it turned out to be difficult to disentangle finite-size effects from a possible crossover in the algebraic exponent. Indeed, the system sizes used in our simulations are much smaller than those used, for example, in Ref. [62]. As a consequence, we did not manage to extract a decay exponent for $\pi_1^u(t)$ which is compatible with the value expected for α within PC universality class. We notice that this is not a peculiarity of this case: such finite volume effects are typically observed in the presence of algebraic decay of correlations, and they occur in equilibrium as well—one example being the Berezinski-Kosterlitz-Thouless phase transition.

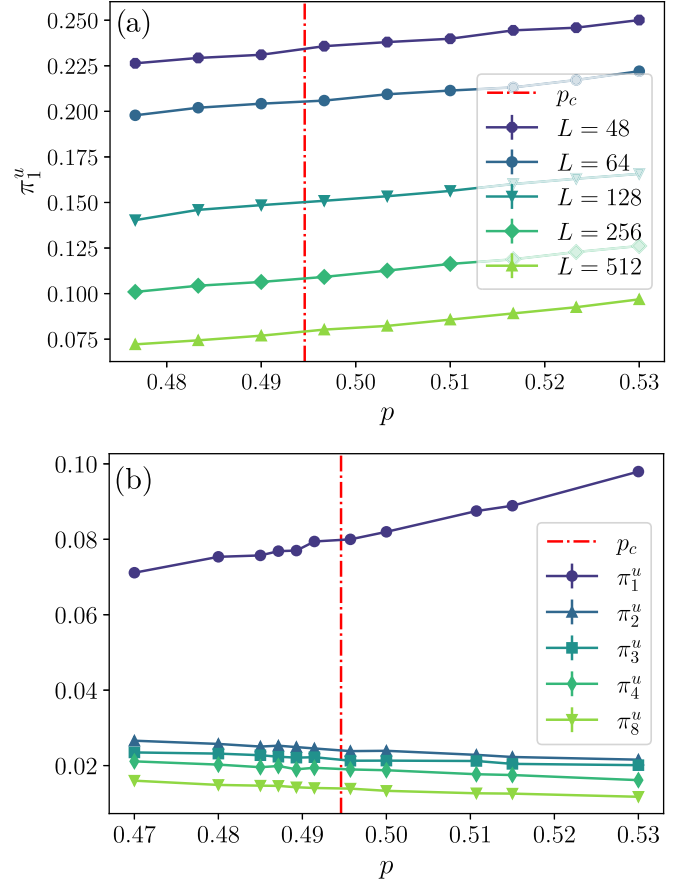


FIG. 10. (a) Largest uncentered normalized eigenvalue π_1^u for BARWe as a function of the probability p , in the vicinity of the critical point $p \simeq p_c$ for various system sizes. Simulations were performed with $N_r = 4000$, and each point is averaged over 20 repetitions. (b) Dependence on p of the first few largest components $\pi_{1,2,3,4,8}^u$ for BARWe, with p close to the critical point p_c and $L = 512$, $N_r = 3000$. Each point is averaged over 10 repetitions.

In Fig. 10(a), we report the steady-state value of π_1^u as a function of the probability p close to the critical point $p \simeq p_c$. In this case, differently from DBP [see Fig. 5(a)], no net change in the normalized spectrum is observed, as shown in Fig. 10. In fact, as p is varied, the largest normalized eigenvalue π_1^u is not affected significantly as it displays a rather smooth behavior also upon increasing L ; see Fig. 10(a). To determine whether the same occurs also to the subleading components, in Fig. 10(b) we plot the dependence on p also of the subsequent eigenvalues $\pi_{2,3,4,8}^u$ for $L = 512$. Differently from DBP, and similarly to what is observed in panel (a) of the same figure, their behavior is still rather smooth upon increasing p and, in addition, no clear quantitative separation emerges among the considered eigenvalues. For example, at the critical point, the first normalized eigenvalue π_1^u is as large as the sum of π_2^u , π_3^u , and π_4^u . Accordingly, we expect that the direct relationship existing between the density and the normalized principal component in the case of DBP might be affected. This ratio displays a different behavior compared to what is observed for DBP, i.e., it does not suddenly approach 1 as p increases beyond p_c . For comparison, note that the plot

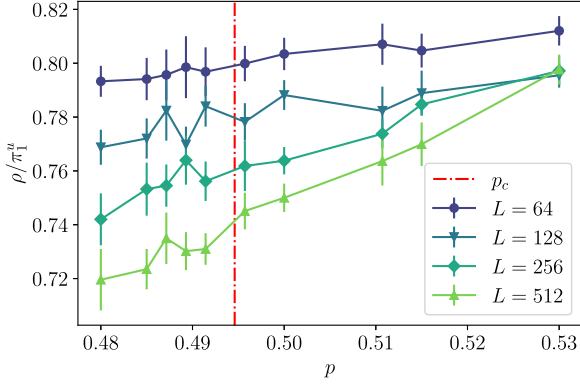


FIG. 11. Dependence of the ratio ρ/π_1^u for BARWe on the probability p , obtained for $N_r = 3000$ and various values of the system size L . Each point is averaged over 10 realizations.

in Fig. 11 spans a significantly wider range of values of p than that for DBP in Fig. 4.

To determine the critical exponents and the critical point, we perform a finite-size scaling analysis on the steady-state values of π_1^u according to Eq. (20), with the result reported in Fig. 12(a). The estimate of the critical value p_* of p which yields the best data collapse is compatible with previous estimates [58]; see also Table I. However, differently from the case of DBP, the corresponding values of the exponents $\omega_* = -0.45(1)$ and $\zeta_* = 0.45(5)$ are not compatible with $-\beta/\nu_\perp = -0.50(2)$ and $1/\nu_\perp = 0.54(2)$ (see Table I), respectively. As we argued previously, this discrepancy might be related to the different structures in the normalized spectrum, in which the subsequent principal components of the PCA do not differ by an order of magnitude from the largest one; see Fig. 10.

To proceed further with our analysis, we also perform a finite-size scaling analysis of the time dependence of $\pi_1^u(t)$ during an evolution with $p = p_c$ [see Eq. (21)], reported in Fig. 12(b). The value $\omega_* = -0.459(3)$ extracted from this analysis is compatible with the value extracted above from the analysis of the steady-state data and thus does not agree with the value $-\beta/\nu_\perp$ expected for PC. Concerning ϕ_* , instead, we find a value $\phi_* = 1.74(3)$ compatible with the dynamical critical exponent 1.7415(5) of the PC universality class (see Table I).

We conclude that, for this model, the similarity between the scaling properties of the particle density ρ and the largest normalized eigenvalue π_1^u is weakened by the fact that the PCA spectrum has a richer structure than in the case of DBP. Nevertheless, some quantities, such as the critical point p_c and the dynamical critical exponent z , can be determined rather accurately with an analysis of the largest principal component.

B. PCA entropies

In analogy with the analysis performed for DBP in Sec. IV C, we analyze here the uncentered Renyi-PCA entropies in Eq. (17) for BARWe. Here we report only the results for the PCA entropy in Eq. (19), while those for the Renyi entropies are discussed in Appendix D. The uncentered PCA entropy S_{PCA}^u in the stationary state of the model as a function

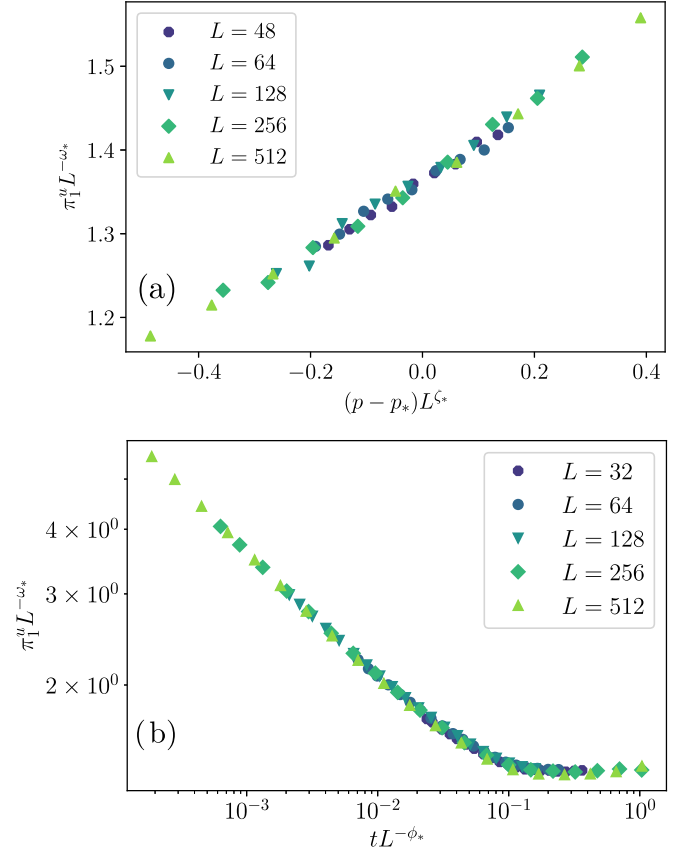


FIG. 12. (a) Finite-size scaling of π_1^u for BARWe in the steady state. The values p_* , ζ_* , and ω_* of the corresponding parameters p_c , ζ , and ω which yield the best data collapse according to Eq. (20) are $p_* = 0.500(9)$, $\zeta_* = 0.45(5)$, $\omega_* = -0.45(1)$. (b) Finite-size scaling analysis of the time dependence of $\pi_1^u(t)$ at the critical point $p = p_c$ (with p_c given in Table I). The values ϕ_* and ω_* of the corresponding parameters ϕ and ω which yield the best data collapse according to Eq. (21) are $\phi_* = 1.74(3)$, $\omega_* = -0.459(3)$. In both cases, simulations were performed for $N_r = 4000$ and each data point is the result of averages over 20 realizations.

of the probability p is reported in Fig. 13 for various system sizes L . The Shannon entropy $S(\rho_S)$ associated with the particle density ρ_S [see Eq. (28)], instead, is reported in Fig. 14. In this case, we find that for system size $L \in [64, 512]$, the PCA entropy develops a peak at a value of p that differs significantly from the critical value p_c (vertical dash-dotted line). At the same time, however, the PCA entropy does not peak deep down in the active phase at $p \simeq 1$, in the point where the density is approximately 0.5, where one would expect the peak of the corresponding entropy of the data set in the mean-field approximation.

VI. CONCLUSIONS

In this work, we explored the use of principal component analysis (PCA) for studying nonequilibrium universality classes. We have shown that PCA can be successfully applied to determine the critical properties of the directed percolation universality class through the analysis of the largest normalized eigenvalue π_1^u of the second moment matrix constructed

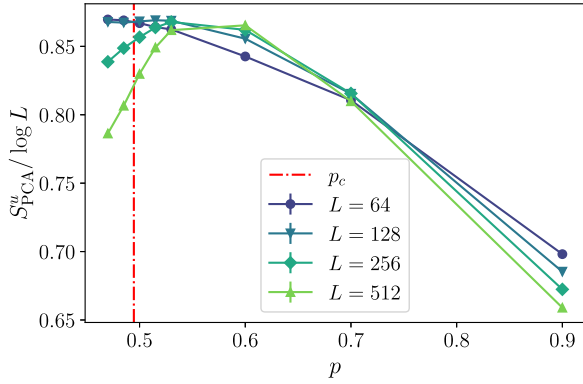


FIG. 13. Normalized uncentered PCA entropy S_{PCA}^u for BARWe, normalized by $\log L$. Simulations were performed with $N_r = 3000$, and each point is the result of an average over 10 repetitions.

from the configuration of the DBP model, either during its evolution or in its stationary state.

In this case, the success of this approach can be attributed to the fact that π_1^u , even close to criticality, is well separated from the smaller eigenvalues. At the same time, we have shown that entropic quantities that keep track of the entire PCA spectrum can serve as indicators of criticality, as shown in the case of DBP (Fig. 7). For models showing a PCA spectrum with a richer structure, such as BARWe, the similarity between the scaling properties of the largest normalized eigenvalue and of the order parameter of the model is considerably weaker—a fact that we attribute to larger finite-volume effects. Nevertheless, some quantities, such as the critical point and the dynamical critical exponent, can still be inferred accurately from the analysis of the sole largest normalized eigenvalue π_1^u . Importantly, we elucidate our numerical observations by employing linear algebra arguments, which form the basis of PCA, thereby leveraging its interpretable nature.

Our findings show an interesting connection with low-rank approximations of data sets. In particular, our observations imply that low-rank (even rank-1) approximations of data

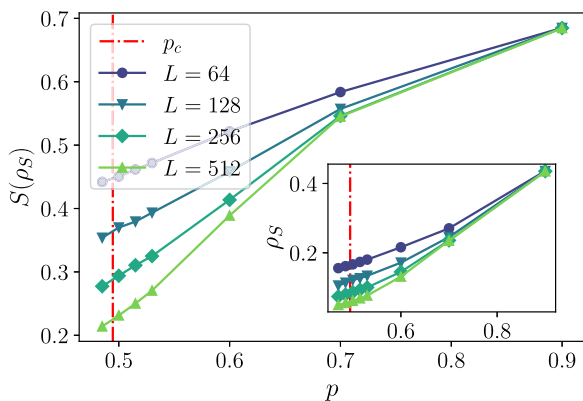


FIG. 14. Shannon entropy of the order parameter as a function of p . For BARWe, $S(\rho_S)$ peaks deep down in the active phase, as $\rho_S = 0.5$ is far from the critical point. Simulations were performed with $N_r = 3000$, and each point is the result of an average of over 10 repetitions.

sets can be successfully used to capture the universality of nonequilibrium phase transitions. This observation has important consequences for experiments since it implies that certain kinds of data sets can be compressed while still preserving universal properties. We note that similar conclusions were drawn concerning random graphs [80].

Some of our arguments hinge upon the binary nature of the data sets. Within this kind of data set, it is plausible that our findings might apply not only to the models considered in this work, but to all models displaying a “dominant” principal component and a phase transition that can be characterized in terms of a uniform order parameter. It would be interesting to see if quantitative statements about rank-1 approximations carry over to models with integer (but nonbinary) or real variables.

The results presented here demonstrate that (linear) dimensional reduction works drastically differently in different universality classes. Investigating how this occurs will likely require taking into account also nonlinear effects. In this direction, possible approaches are provided by the kernel analysis, or even by a full data structure characterization based on network theory, which, so far, have been only applied to models at equilibrium [69,81,82].

ACKNOWLEDGMENTS

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APPENDIX A: CENTERED PCA ANALYSIS

In this appendix, we report the analysis of the centered entropies, focusing on the PCA entropy S_{PCA}^c and on the Renyi-PCA entropy of order 2, i.e., $S_{\text{PCA},2}^c$ defined on the basis of the centered spectrum $\{\pi_i^c\}$ in Eqs. (17) and (19), respectively. We first discuss these quantities for the case of DBP, finding that they are also informative about the transition. In particular, the centered PCA entropy S_{PCA}^c can be used to locate the critical point. This is shown in Fig. 15, which reports S_{PCA}^c as a function of p close to the expected critical value, and for various values of the system size L . Differently from what happens for S_{PCA}^u , the centered PCA entropy S_{PCA}^c does not display a peak close to the critical point, but only features a crossing of the various curves for different values of system size. Similar behavior is observed also in the PCA-Renyi 2 entropy $S_{\text{PCA},2}^c$, as shown in Fig. 16.

The behavior of S_{PCA}^c and $S_{\text{PCA},2}^c$ for the BARWe is shown in Figs. 17 and 18, respectively. In this case, no crossing is observed in these quantities, when normalized in the same fashion, i.e., by $\log L$. This might be related to the richer structure that the PCA spectrum has for BARWe, which was also observed for the corresponding uncentered quantities discussed in Sec. VA of the main text.

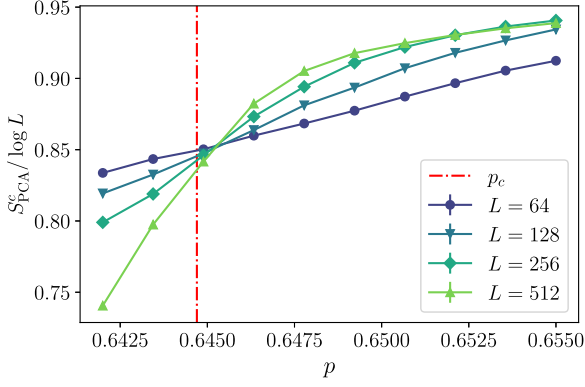


FIG. 15. Centered normalized PCA entropy S_{PCA}^c as a function of p in the vicinity of the critical point for DBP and various values of the system size L . The curves corresponding to the various L cross each other close to criticality. Simulations correspond to $N_r = 2000$ and each point is averaged over five repetitions.

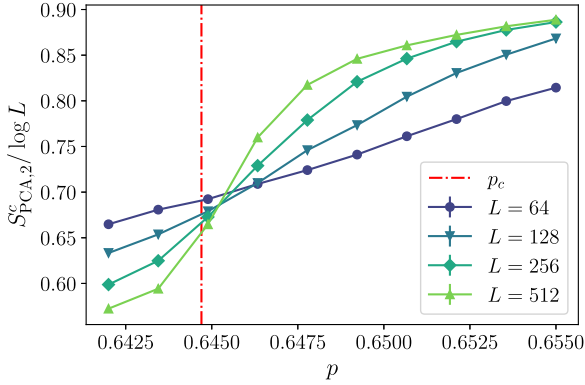


FIG. 16. Centered normalized PCA-Renyi 2 entropy $S_{\text{PCA},2}^c$ in the vicinity of the critical point for DBP and various values of the system size L . The curves corresponding to the various L cross each other close to criticality, as it occurs for S_{PCA}^c in Fig. 15. Simulations correspond to $N_r = 2000$ and each point is averaged over five repetitions.

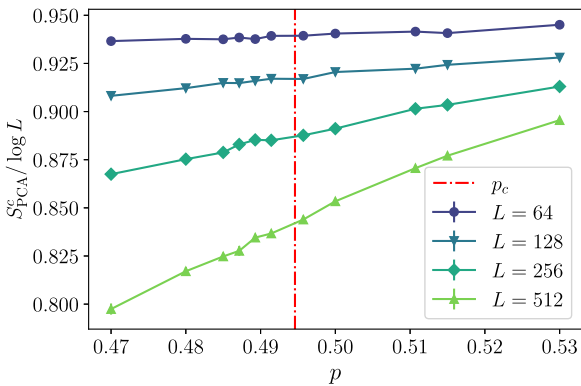


FIG. 17. Centered normalized PCA entropy S_{PCA}^c as a function of p in the vicinity of the critical point for BARWe and various values of the system size L . Differently from the case of directed percolation shown in Fig. 15, no crossing is observed. Simulations correspond to $N_r = 3000$, and points are averaged over 10 repetitions.

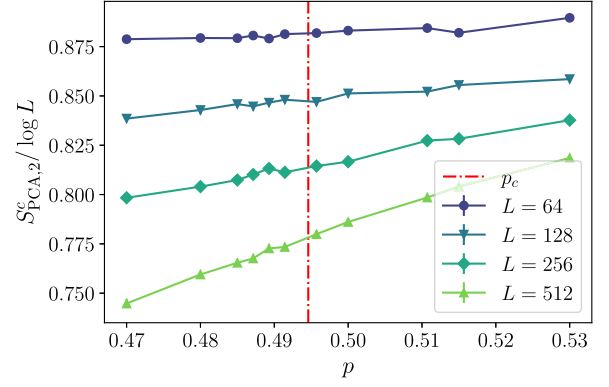


FIG. 18. Centered normalized PCA-Renyi 2 entropy $S_{\text{PCA},2}^c$ in the vicinity of the critical point for BARWe and various values of the system size L . Differently from the case of directed percolation shown in Fig. 16, no crossing is observed. Simulations correspond to $N_r = 3000$, and points are averaged over 10 repetitions.

APPENDIX B: QUANTIFIED PRINCIPAL COMPONENTS

The analyses presented in the main text of this work and in the previous appendices were based on doing a PCA on the data matrix \mathbf{X} [see the definition in Eq. (12)], which collects various configurations of the system at a given value of p (in the steady state) or at a given p and time t (during relaxation). Here, we discuss a complementary type of analysis in which one collects all available data into a single data matrix. Let us illustrate the procedure for the case of data sets in the steady state. For a fixed system size L , we collect the data matrices \mathbf{X} (constructed as explained in Sec. III) corresponding to each single value of p , which, for clarity, we denote by \mathbf{X}_p . Then we consider the data set formed by the matrices \mathbf{X}_p corresponding to all the values of p which are considered in the analysis, i.e., $\{\mathbf{X}_p\}$, and we collect all these observations into a single data matrix, which we denote by \mathbf{Y} . This data matrix has the same number of columns (corresponding to the number of lattice sites) as the individual matrices \mathbf{X}_p . However, the number of rows is now $N_r \times N_p$ (instead of N_r), where N_p is the number of values of the control parameter p probed by the simulations. We then performed a column-centered PCA on \mathbf{Y} [as in Eq. (13) with $\mathbf{X} \mapsto \mathbf{Y}$ and $N_r \mapsto N_r \times N_p$] and looked at the information contained in the eigenvectors of the covariance matrix of \mathbf{Y} [see Eq. (14)]. More concretely, following Ref. [17], we define the *quantified principal components* (QPCs) as the average of the inner product of the data points corresponding to a given p with the L -dimensional normalized eigenvectors \vec{w}_i of the covariance matrix associated with \mathbf{Y} . Accordingly, the QPCs are given by

$$\langle |\text{PC}_i| \rangle(p) := \frac{1}{N_r} \sum_{\mu=1}^{N_r} |\vec{x}^{(\mu)}(p) \cdot \vec{w}_i|, \quad (\text{B1})$$

where $\vec{x}^{(\mu)}(p)$ are the L -dimensional row vectors in \mathbf{X}_p .

The first two QPCs, i.e., $\langle |\text{PC}_1| \rangle$ and $\langle |\text{PC}_2| \rangle$, for the stationary behavior (with the system configurations being sampled at a fixed time $t = L^\tau$) of DBP, are shown in Figs. 19 and 20, respectively (the corresponding results are averaged over 10 independent repetitions). For each value of p , we used

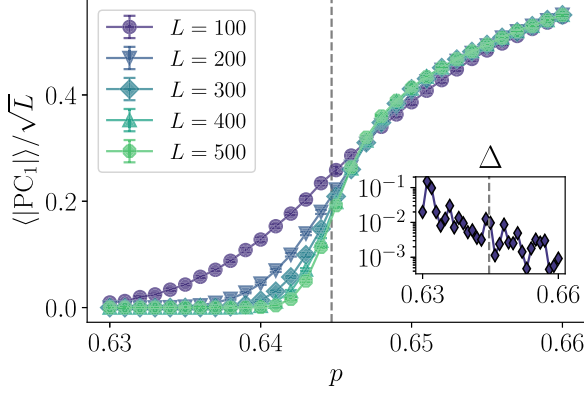


FIG. 19. First QPC $\langle |PC_1| \rangle$ for DBP in the stationary state. We take $N_r = 1000$ for each value of p . The inset shows the relative difference Δ defined in Eq. (B3) between the density ρ of active sites and the first QPC for $L = 100$ (similar behavior is observed for other values of L). This demonstrates a quantitative agreement between the two quantities across the considered range of values of the control parameter. The dashed line indicates the position of the critical point $p_c \approx 0.6447$.

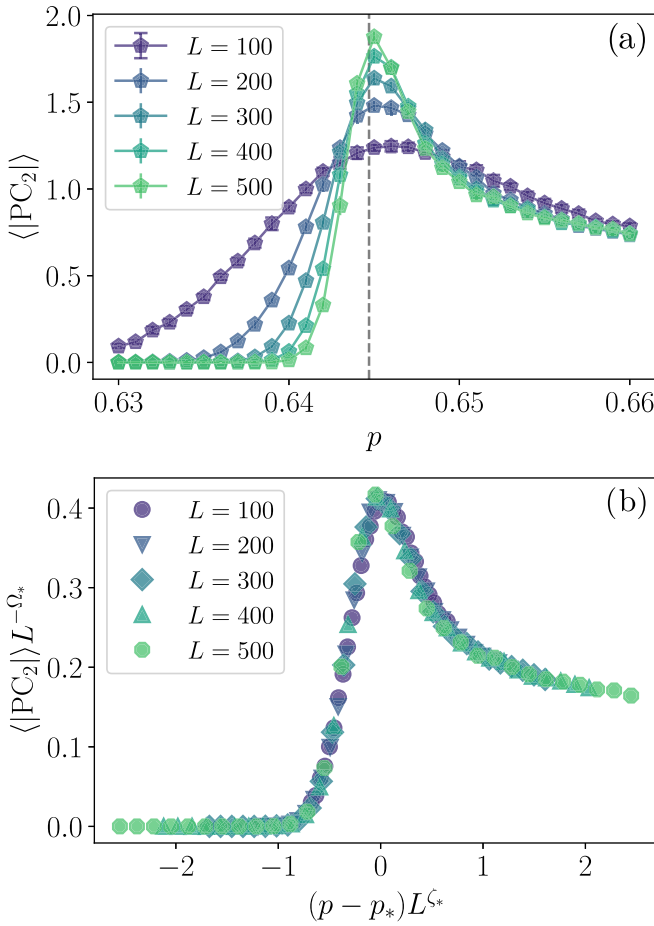


FIG. 20. (a) Second QPC $\langle |PC_2| \rangle$ for DBP in the stationary state, which shows a clear signature of the transition point as the system size is increased. The various remaining parameters take the same values as in Fig. 19. (b) Finite-size scaling of the second QPC in the stationary state. The obtained critical point and exponents that realize the data collapse are given by $p_* = 0.64484(5)$, $\Omega_* = 0.261(4)$, $\zeta_* = 0.90(1)$.

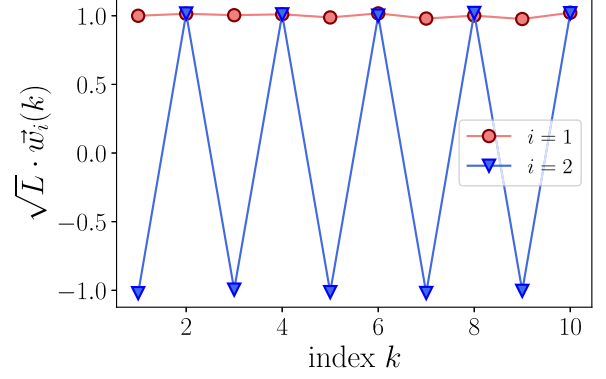


FIG. 21. Entries of the first two normalized eigenvectors of \mathbf{Y} as a function of the entry index k for the steady-state analysis of DBP with $L = 100$. Only the first 10 entries of these L -dimensional vectors are shown here for clarity, but the same structure is observed for the remaining entries of both eigenvectors. The same behavior occurs irrespective of the value of L (up to numerical variations).

$N_r = 1000$. These figures reveal that the critical properties of the model are contained also in the eigenvectors of the covariance matrix associated with the data matrix \mathbf{Y} . In particular, we observe that the first QPC, rescaled by a factor of \sqrt{L} , captures quantitatively the behavior of the order parameter ρ (see Fig. 19). This can be understood from the numerical observation that, for the system under consideration, the structure of the first eigenvector \bar{w}_1 is roughly homogeneous, namely, $\bar{w}_1 \approx \frac{1}{\sqrt{L}}(1, 1, \dots, 1)$. This is shown in Fig. 21, which reports the first 10 entries of \bar{w}_1 and \bar{w}_2 . Hence, because of the definition of $\langle |PC_1| \rangle$ in Eq. (B1), its connection to the order parameter is clear, namely,

$$\langle |PC_1| \rangle(p) \approx \frac{1}{N_r} \frac{1}{\sqrt{L}} \sum_{\mu=1}^{N_r} \sum_{i=1}^L x_i^{(\mu)}(p) \approx \sqrt{L} \rho(p), \quad (\text{B2})$$

where $\rho(p)$ is the stationary density at a given p .

In the inset of Fig. 19, we plot the relative difference Δ between the particle density ρ and $\langle |PC_1| \rangle / \sqrt{L}$, i.e.,

$$\Delta := \left| \frac{\rho - \langle |PC_1| \rangle / \sqrt{L}}{\rho} \right| \quad (\text{B3})$$

for $L = 100$ (similar behavior is observed for other values of L). This difference turns out to be always rather small, independently of the value of p , as expected from Eq. (B2).

The second QPC $\langle |PC_2| \rangle$ in Fig. 20(a) clearly signals the onset of the phase transition in a fashion that closely resembles the behavior of a susceptibility for a system at equilibrium featuring a continuous (second-order) phase transition. Note that $\langle |PC_2| \rangle$ is reminiscent of a staggered density (see \bar{w}_2 in Fig. 21) and, to our knowledge, it has not been previously examined for the DBP. Accordingly, the fact discussed below that it displays an interesting scaling behavior can be considered a genuine discovery of the PCA. To test if this quantity has good scaling properties, we perform a finite-size scaling with the ansatz

$$\langle |PC_2| \rangle(p) = L^{\Omega} h((p - p_c)L^{\zeta}). \quad (\text{B4})$$

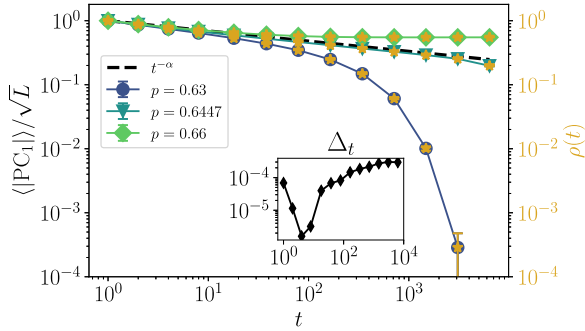


FIG. 22. First QPC $\langle |PC_1| \rangle$ for DBP during relaxation from a fully active initial state, for $L = 256$, and $N_r = 1000$ (for each value of t). The \star markers show the density $\rho(t)$ of active sites (the corresponding scale is shown along the vertical axis on the right side of the plot), showing a quantitative agreement between the two quantities. The inset shows the value Δ_t of the relative difference Δ [see Eq. (B3)] between the density $\rho(t)$ of active sites and $\langle |PC_1| \rangle / \sqrt{L}$ at $p = 0.6447$. This demonstrates a quantitative agreement between the two quantities across the considered range of evolution times.

As shown in Fig. 20(b), $\langle |PC_2| \rangle$ exhibits good scaling properties, which is made explicit by the collapse of data for different system sizes onto a master curve h . The values of the critical point and of the exponents that yield the best data collapse are $p_* = 0.64484(5)$, $\Omega_* = 0.261(4)$, $\zeta_* = 0.90(1)$. Remarkably p_* and ζ_* are good estimates for the expected values of p_c and $1/\nu_\perp$. Concerning Ω_* , it appears that $\Omega_* \approx -\omega_*$ (with ω_* reported in the main text in Sec. IV).

The same analysis can also be applied to the data concerning the time evolution of the system, where now we collect all the available data at various times during the evolution (at fixed p). Figure 22 shows $\langle |PC_1| \rangle$ as a function of t for various values of p and $L = 256$. At each time t , we collect $N_r = 1000$ configurations. We show the results after averaging over 10 independent runs. This plot also shows the corresponding value of the time-dependent density of active sites $\rho(t)$ (\star markers), which is practically indistinguishable from $\langle |PC_1| \rangle$ (rescaled by \sqrt{L}). This also follows from the structure of the first normalized eigenvector \bar{w}_1 , which, just as for the static case, is roughly homogeneous, i.e., $\bar{w}_1 \approx \frac{1}{\sqrt{L}}(1, 1, \dots, 1)$. The inset in this figure shows the time-dependent value Δ_t of the quantity Δ defined in Eq. (B3), plotted as a function of time t , for the data corresponding to $p = 0.6447$. This relative difference turns out to be smaller than $\approx 10^{-3}$. It is thus clear that even when considered in the time domain, $\langle |PC_1| \rangle$ reproduces quantitatively the behavior of the order parameter.

APPENDIX C: FINITE-SIZE SCALING

As a starting point for our discussion, let us consider a system at thermal equilibrium that undergoes a continuous phase transition upon tuning the value of a parameter g to its critical value g_c . Accordingly, in the thermodynamic limit, the correlation length of the order parameter fluctuations within

the system for $g \rightarrow g_c$ increases as

$$\xi \sim |g - g_c|^{-\nu}, \tag{C1}$$

where ν is the critical exponent associated with the universality class to which the system under consideration belongs. Now, let us consider a quantity O which, in the thermodynamic limit, displays a singularity of the form

$$O \sim |g - g_c|^{\gamma_O}, \tag{C2}$$

where γ_O is an exponent depending on O . If the system has a finite spatial extent of typical size L , the singularities mentioned above are replaced by a regular behavior as a function of g predicted by the finite-size scaling theory at equilibrium [83,84]. In particular, for $g \rightarrow g_c$ and sufficiently large L , Eq. (C2) is replaced by

$$O(g, L) = L^{-\gamma_O/\nu} \tilde{O}((g - g_c)L^{1/\nu}), \tag{C3}$$

where \tilde{O} is a scaling function independent of the system size L . This scaling ansatz actually provides a method for determining both the critical exponents and the critical point. In fact, if the critical point g_c and the exponents γ_O and ν associated with the transition are known, plotting $L^{\gamma_O/\nu} O(g, L)$ as a function of $(g - g_c)L^{1/\nu}$ should result in a collapse of the data concerning the dependence of O on g for various systems sizes L , because the scaling function \tilde{O} is independent of L (at least at the leading order as L grows). Accordingly, one can reverse the argument and determine the critical exponents and the critical point by treating ν , γ_O , and g_c as fitting parameters and by estimating them with the corresponding values ν_* , γ_* , and g_* which yield the best data collapse onto a single master curve. For example, this might amount to minimizing some distance between the scaled data. To perform the finite-size scaling, we adopt the method described in Ref. [74]. The same scaling form as Eq. (C3) and its generalizations can be used to describe steady-state scaling observables for nonequilibrium phase transitions [85]. For every scaling quantity O depending on the parameter p (see Sec. II) and in a finite volume of size L , one can assume a scaling form

$$O(p, L) = L^\omega \tilde{O}((p - p_c)L^\zeta), \tag{C4}$$

where ω and ζ could, in principle, depend on the quantity O taken into consideration, i.e., $\omega = \omega_O$ and $\zeta = \zeta_O$. However, in an ideal scenario in which the (stationary and dynamic) properties of the system are actually controlled by a well-defined and growing correlation length, the exponent ζ should actually be independent of the observable and be fixed to $1/\nu$ [where ν is defined in Eq. (C1)], especially when the quantity under study displays a favorable scaling behavior.

We now briefly describe the approach we used for obtaining and optimizing the data collapse in the finite-size scaling analysis, following Ref. [74]. The method consists in minimizing a cost function that is computed on the basis of the raw numerical data for $O(p, L)$ and the associated error $\sigma_O(p, L)$, expressed in terms of the scaled variables $x \equiv (p - \bar{p}_c)L^\zeta$, $y \equiv OL^{-\omega}$ and scaled errors $\sigma = \sigma_O L^{-\bar{\omega}}$, where $\bar{\zeta}$, $\bar{\omega}$ are the candidate scaling exponents, and \bar{p}_c is the candidate critical value of p . The scaled data and errors are computed for all the values $\{L_k\}_{k=1}^{N_L}$ of the system size L and for all the values $\{p_j\}_{j=1}^{N_p}$ of the probability p considered in the numerical study.

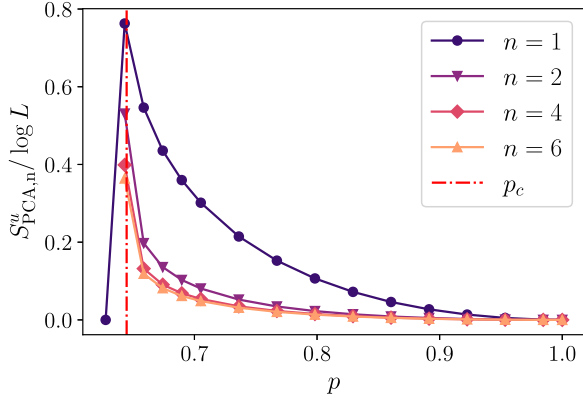


FIG. 23. Uncentered Renyi-PCA entropies $S_{\text{PCA},n}^u$ as a function of p for DBP and various values of n . The numerical data are obtained for $L = 512$, $N_r = 3000$. Each data point is averaged over five repetitions.

The resulting set $\{(x_i, y_i, \sigma_i)\}_{i=1}^n$ of $n = N_L \times N_p$ scaled data is then ordered such that $x_i < x_{i+1}$. The best estimates p_* , ω_* , and ζ_* for the critical point p_c and the scaling exponents $\bar{\omega}$ and $\bar{\zeta}$, respectively, are obtained as the arguments that minimize the cost (or quality) function

$$Q(\bar{p}, \bar{\omega}, \bar{\zeta}) = \sum_{i=2}^{n-1} \frac{w(x_i, y_i, \sigma_i | x_{i-1}, y_{i-1}, \sigma_{i-1}, x_{i+1}, y_{i+1}, \sigma_{i+1})}{n-2}, \quad (\text{C5})$$

where

$$w(x, y, \sigma | x', y', \sigma', x'', y'', \sigma'') = \frac{(y - \bar{y})^2}{\Delta^2} \quad (\text{C6})$$

are the square distances of the point (x, y) from the point (x, \bar{y}) obtained from a linear interpolation of the preceding and following data points, i.e., (x', y') and (x'', y'') , respectively, in units of the error Δ on $y - \bar{y}$. In formulas

$$\bar{y} = \frac{(x'' - x)y' - (x' - x)y''}{x'' - x'}, \quad (\text{C7})$$

while Δ is obtained by a standard propagation of errors, i.e.,

$$\Delta^2 = \sigma^2 + \left(\frac{x'' - x}{x'' - x'} \sigma' \right)^2 + \left(\frac{x' - x}{x'' - x'} \sigma'' \right)^2. \quad (\text{C8})$$

Error bars [86] are assigned according to the method of Ref. [86]. If we have to perform the minimization of Q on a set of N_L curves, we consider all N_L subsets composed by $N_L - 1$ different curves and estimate, for each subset, the exponents and p_* as explained above. The critical exponents and p_* for the whole set of data are then estimated as the mean of the N_L

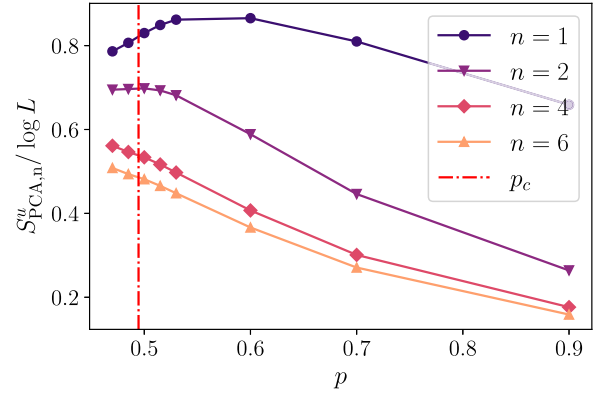


FIG. 24. Uncentered Renyi-PCA entropies $S_{\text{PCA},n}^u$ as a function of p for BARWe and various values of n . The numerical data are obtained for $L = 512$, $N_r = 3000$. Each data point is averaged over 10 repetitions.

previous estimates. As the values extracted from each subset are expected to be correlated and an accurate determination of the resulting error would thus require a more complex analysis beyond what is needed here, we simply assign as an error on the final estimates their standard deviations instead of those of their means.

APPENDIX D: RENEYI-PCA ENTROPIES

In this appendix, we report the behavior of uncentered Renyi-PCA entropies $S_{\text{PCA},n}^u$ defined in Eq. (17). As discussed in Sec. IV C of the main text for DBP, the peak in the PCA entropy [see Eq. (19)] provides a good estimate of the critical point. A similar behavior is displayed by $S_{\text{PCA},n}$ for generic n , as shown in Fig. 23. Upon increasing n , the values of these Renyi entropies are increasingly determined by the first few largest components of the PCA spectrum $\{\pi_i^u\}$. This indicates that, consistently with what was observed in Sec. IV A, most of the information about the transition is actually encoded in the behavior of the largest component. As discussed in the main text in Sec. V A, the case of BARWe is complicated by a richer structure in the PCA spectrum which affects also the behavior of the corresponding $S_{\text{PCA},n}^u$. This is shown for the various $S_{\text{PCA},n}^u$ in Fig. 24. Upon increasing n , we observe that the peak of $S_{\text{PCA},n}$ in the active phase disappears and the curves become monotonic. While S_{PCA} features a local maximum above p_c , due to the relevant contributions coming from the various components of the spectrum beyond π_1^u , $S_{\text{PCA},n}^u$ increasingly mirrors the behavior of π_1^u . However, even the behavior of π_1^u does not provide as much clear information about the occurrence of the phase transition as in the case of DBP.

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