Field-theoretic approach to metastability in the contact process

Christophe Deroulers[1,*] and Rémi Monasson[2,3,†]
[1]*Laboratoire de Physique Théorique de l'ENS, 24 rue Lhomond, 75231 Paris CEDEX 05, France*
[2]*CNRS–Laboratoire de Physique Théorique de l'ENS, 24 rue Lhomond, 75231 Paris CEDEX 05, France*
[3]*CNRS–Laboratoire de Physique Théorique, 3 rue de l'Université, 67000 Strasbourg, France*
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A "quantum" field-theoretic formulation of the dynamics of the contact process on a regular graph of degree z is introduced. A perturbative calculation in powers of $1/z$ of the effective potential for the density of particles $\phi(t)$ and an instantonic field $\psi(t)$ emerging from the formalism is performed. Corrections to the mean-field distribution of densities of particles in the out-of-equilibrium stationary state are derived in powers of $1/z$. Results for typical (e.g., average density) and rare fluctuation (e.g. lifetime of the metastable state) properties are in very good agreement with numerical simulations carried out on D-dimensional hypercubic ($z=2D$) and Cayley lattices.

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I. INTRODUCTION

A. Motivations

Recent years have seen an upsurge of interest for the dynamical properties of out-of-equilibrium systems in statistical physics [1]. Systems of interacting elements are ubiquitous in physics and other fields, e.g., biology, computer science, economy, etc. Most of the time the dynamical rules do not obey detailed balance or similar criteria which would ensure the existence of a well defined stationary distribution at large times. In other cases, a Gibbs measure does exist but is out of reach on experimental time scales, and all phenomena of interest, e.g., the occurrence of dynamical phase transitions take place when the system is truly out of equilibrium. An example of such out-of-equilibrium phenomena, frequently encountered in condensed matter, in cellular automata or even in computationally motivated problems is the occurrence of metastable states, or regions in phase space in which trapping may take place for a very long time before further evolution becomes possible.

The calculation of the temporal properties of these systems often turns out to be very hard, even when dynamical rules look like innocuously simple. Over the past decade, however, various models and problems have been successfully investigated, e.g., Refs. [2–6]. Among the analytical methods used to tackle these systems, some rely on the observation that the master equation for a system of classical degrees of freedom may be seen as a Schrödinger equation (in imaginary time) where the quantum Hamiltonian encodes the evolution operator. Exact, e.g., Bethe ansatz [3] or approximate, e.g., variational or semiclassical techniques developed in the context of quantum field theory may be used to understand the dynamical properties of the original system [7]. One important achievement made possible by this approach once combined with renormalization group techniques has been the calculation of decay exponents and the identification of universality classes in reaction-diffusion models [8,9].

The range of this "quantum" procedure is however not limited to the calculation of universal quantities. In this work, we show how it can be combined with diagrammatic techniques developed in the contexts of field theory and the statistical physics of disordered systems to quantitatively characterize the metastable properties of a well-known example of out-of-equilibrium system, the so-called contact process (CP) [10]. In spite of its technicalities, this approach allows us to make predictions that can be successfully compared to numerical simulations. It is expected that it will permit to investigate metastability [11,12], or other properties of various dynamical models.

B. The contact process: Definition and phenomenology

We consider a regular graph G with vertex degree z and size N (number of vertices). Each vertex (or node, or site) may be empty or occupied by one particle. Hereafter, we focus on the continuous time version of CP where a particle is spontaneously annihilated with rate 1 independently from other sites, and an empty site becomes occupied with rate $\lambda n_{\mathrm{occ}}/z$ where n_{occ} is the number of its occupied nearest neighbors [10].

The value of the parameter λ strongly affects the behavior of CP. For infinite size graphs, e.g., infinite hypercubic lattices, there exists a critical value λ_C of λ such that [13] the following hold.

(1) If $\lambda<\lambda_C$, the number of particles (occupied sites) quickly decreases towards zero. Later, the system remains trapped in this empty configuration.

(2) If $\lambda>\lambda_C$, the density ρ of particles reaches a plateau value $\rho^*(\lambda)$ independently on the initial density [14].

(3) At criticality, that is, when $\lambda=\lambda_C$, the density eventually relaxes to zero with a slow algebraic decay $\rho(t) \sim t^{-a}$. This critical behavior falls into the directed percolation universality class [15–17]. Exponent a is equal to 1 in dimensions larger than $D_c=4$, and approximate expressions in powers of D_c-D in lower dimensions have been obtained

*Electronic address: Christophe.Deroulers@ens.fr
†Electronic address: monasson@lpt.ens.fr

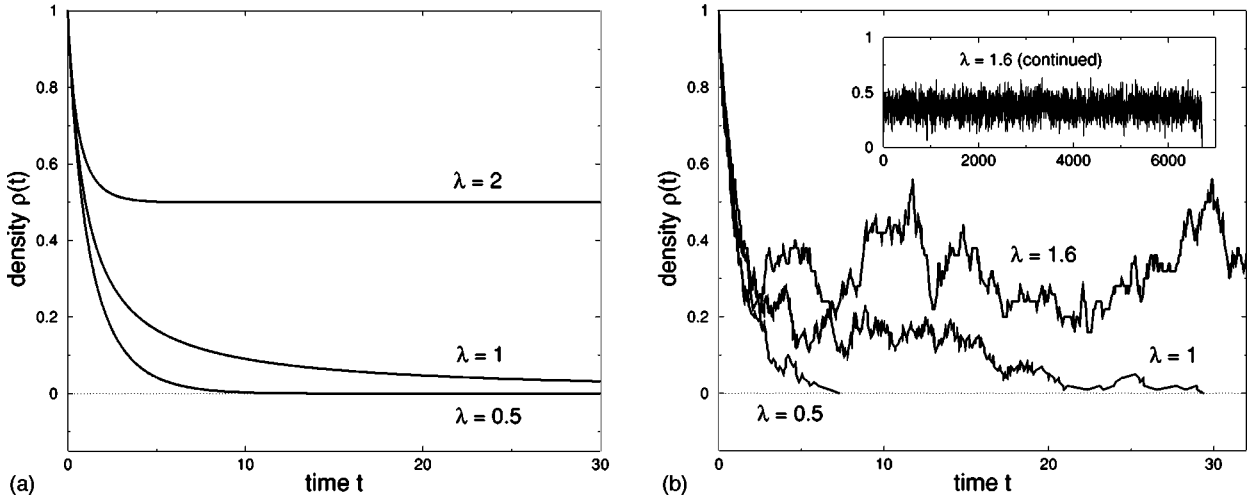

FIG. 1. Profiles of the density ρ of particles vs time t for the contact process over a complete graph of N vertices, initially filled with particles [$\rho(0)=1$]. (a). Thermodynamic limit, $N\to\infty$. From bottom to top: subcritical ($\lambda<\lambda_C=1$, the density exponentially relaxes toward zero), critical ($\lambda=\lambda_C$, the density algebraically decays to zero as $\rho(t)\sim t^{-1}$), and supercritical ($\lambda>\lambda_C$, the density exponentially relaxes to a finite value, $\rho^*=1-1/\lambda$) cases. The density obeys a deterministic evolution equation (36), and no fluctuation is present. (b). Finite size lattice, with $N=100$ sites. CP is a stochastic process, and the density profiles vary from run to run (we show here one run for each value of λ). The density quickly relaxes to zero (subcritical regime) or a finite value (supercritical regime). In the latter case, the system is trapped in a metastable regime where the density fluctuates for a very long time around its plateau value (inset: notice the difference of time scale), till a large fluctuation drives the density to the zero value.

through the use of renormalization group techniques [7–9,15–18].

These behaviors are displayed in Fig. 1(a). The exact value of the critical parameter λ_C is unknown in any dimension D, but rigorous bounds and estimates have been derived [13(b)].

For finite-size graphs, the empty configuration, referred to as vacuum in the following, is an absorbing state for the dynamics. Starting from any initial configuration, e.g., fully occupied state, CP will eventually end up in the vacuum configuration after a finite time t_{vac}. This forces the above infinite-size picture to be smeared out by fluctuations in the case of large but finite lattices [11,13(b),19]. λ_C locates a cross-over between fast [$t_{vac}(N,\lambda<\lambda_C)=O(\ln N)$] and very slow [$t_{vac}(N,\lambda>\lambda_C)\sim\exp O(N)$] relaxations towards the vacuum configuration. In the latter regime, the plateau height ρ^* merely defines an average value around which the density exhibits fluctuations until the system is driven to the vacuum through a very large fluctuation [Fig. 1(b)]. On time scales $1\ll t\ll t_{vac}(N,\lambda>\lambda_C)$, the system is trapped into a metastable state [20]. A (pseudo)equilibrium probability measure for the density can be defined,

$$P(\rho,N)=\exp[N\,\pi^*(\rho)+o(N)]. \tag{1}$$

Function π^*, which depends on λ and other parameters, e.g., the dimension D for hypercubic lattices, describes rare fluctuations from the average density ρ^*. Its maximal value is zero for $\rho=\rho^*$. Densities ρ distinct from the average one are exponentially (in N) unlikely to be reached, and $\pi^*(\rho)<0$, see Fig. 2. In particular, the probability of a very large fluctuation annihilating all particles scales as $\exp[N\pi^*(0)]$, and thus,

$$t_{vac}(N)=\exp[-N\pi^*(0)+o(N)]. \tag{2}$$

The calculation of the large deviation function $\pi^*(\rho)$ is the main scope of this paper. For this purpose we use a path-

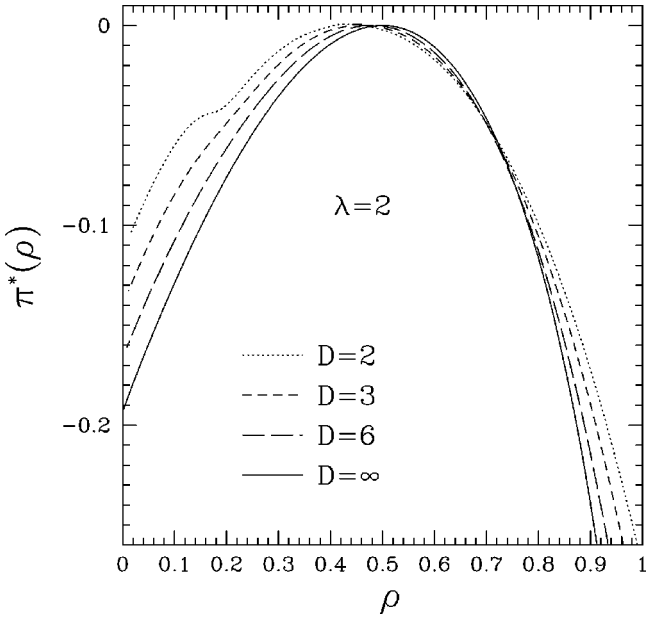

FIG. 2. The large deviation function π^* for the density of particles in CP with parameter $\lambda=2$ for the D-dimensional hypercubic lattice. The $D\to\infty$ curve corresponds to the mean-field limit, and coincides with the case of the complete graph over $N\to\infty$ sites. Plots of the predicted value of $\pi^*(\rho)$ at the order $1/D$ for $D=6$, 3, and 2 are obtained with the expansion of Sec. IV. The nonconvexity of the curve for $D=2$ shows the inaccuracy of the truncation to first order of our $1/D$ expansion in this range of densities.

integral representation of π^* where particles are encoded into quantum hard-core bosons, or $\frac{1}{2}$ spins, and develop a diagrammatic self-consistent evaluation of the path integral which allows us to write a systematic expansion of π^* in powers of $1/z$ (Sec. II). In the infinite connectivity limit ($z \to \infty$), this formalism reduces to the mean-field theory of CP, analyzed in Sec. III. Finite connectivity corrections to π^* are calculated in Sec. IV. As a by-product, we obtain an expansion for the critical parameter $\lambda_C(z)$ in powers of $1/z$. The validity of our calculation, effectively carried out up to order $1/z^2$ (and $1/z$ for π^*), is confirmed by numerical simulations performed on D-dimensional hypercubic ($z=2D$) and Cayley lattices.

II. FIELD-THEORETIC FRAMEWORK

A. Path-integral formulation of the evolution operator

We start by writing the master equation of CP using a quantum formalism, according to the familiar procedure of Felderhof, Doi, and successors [21,22]. For each site i of the graph we define a hard-core boson with associated state vectors $|0\rangle_i$ (empty) and $|1\rangle_i$ (occupied), and creation and annihilation operators $a_i^\dagger$ and a_i that anticommute on a single site but commute on different sites: $[a_i, a_i^\dagger]_+ = \mathbb{1}$, $[a_i^\dagger, a_j^\dagger] = [a_i, a_j^\dagger] = [a_i, a_j] = 0$ (alternately, we could use spins 1/2 with a mere rewriting of the equations). To each occupation number $s_i = 0,1$ of site i is associated a vector $|s_i\rangle$. Then, to each state $\vec{s}$ of the graph [set $(s_1, s_2, \ldots, s_N)$ of occupation numbers of all the sites] corresponds [23] a basis vector of a 2^N-dimensional vector space, $|\vec{s}\rangle = |s_1\rangle \otimes |s_2\rangle \otimes \cdots \otimes |s_N\rangle$, and, to the time-dependent probability distribution $P(\vec{s},t)$, the state vector $|P(t)\rangle = \Sigma_{\vec{s}} P(\vec{s},t)|\vec{s}\rangle$. The master equation for $P(\vec{s},t)$ is now equivalent to the evolution equation of the state vector

$$\frac{d}{dt}\Big| P(t)\rangle = \hat{W}|P(t)\rangle, \tag{3}$$

where the evolution operator $\hat{W}$ is the infinitesimal generator of the transitions. For CP, $\hat{W} = \hat{W}_{\text{ann}} + \lambda \hat{W}_{\text{cre}}$ with

$$\hat{W}_{\text{ann}} = \sum_i (\mathbb{1} - a_i^\dagger) a_i,$$

$$\hat{W}_{\text{cre}} = \frac{1}{z} \sum_i \sum_{j \in i} [a_j^\dagger (\mathbb{1} + a_j) - \mathbb{1}] a_i^\dagger a_i, \tag{4}$$

where $j \in i$ means that site j is one of the z nearest neighbors of site i.

To map the stochastic process onto a path integral or field-theoretic formulation [8,9,24], we introduce [25,26] continuously parametrized states suitable for hard-core bosons [27]. On each site of the graph, the state bra and ket are, respectively,

$$\langle \phi, \theta| = (1-\phi)^{1/2} \langle 0| + \phi^{1/2} \exp(-\hat{\imath}\theta) \langle 1|,$$

$$|\phi, \theta\rangle = (1-\phi)^{1/2} |0\rangle + \phi^{1/2} \exp(\hat{\imath}\theta) |1\rangle, \tag{5}$$

TABLE I. Translation table from operators in $\hat{W}$ into Lagrangian contribution to $\tilde{W}$. We have added $aa^\dagger$ in the left column though this operator is not in normal order to show the consistency of the translation rules with the anticommutation relation.

Operator in $\hat{W}$	Expression in $\tilde{W}$
$\mathbb{1}$	1
a	$\phi \exp(\psi)$
$a^\dagger$	$(1-\phi)\exp(-\psi)$
$a^\dagger a$	ϕ
$aa^\dagger$	$1-\phi$

where $\phi \in [0,1]$, $\theta \in [0, 2\pi]$, and $\hat{\imath}^2 = -1$. These states satisfy the closure relation

$$\frac{1}{\pi} \int_0^1 d\phi \int_0^{2\pi} d\theta |\phi, \theta\rangle\langle \phi, \theta| = \mathbb{1}. \tag{6}$$

To allow a simplification of the expressions in the translation table given below, we make use of $\psi := -\frac{1}{2} \ln[\phi/(1-\phi)] + \hat{\imath}\theta$ instead of θ, and introduce the following notations:

$$\langle \phi, \psi| = (1-\phi)^{1/2} [\langle 0| + \exp(-\psi) \langle 1|],$$

$$|\phi, \psi\rangle = (1-\phi)^{-1/2} [(1-\phi)|0\rangle + \phi \exp(\psi)|1\rangle]. \tag{7}$$

For the whole graph, a state is the tensor product of the states over all sites: $|\vec{\phi}, \vec{\psi}\rangle = \otimes_{i=1}^N |\phi_i, \psi_i\rangle$. Making use of Trotter formula [28] and of the closure identity (6), we obtain a path-integral expression for the matrix elements of the evolution operator $\exp(T\hat{W})$ between times 0 and T [8,24],

$$\langle \vec{\phi}_T, \vec{\psi}_T | \exp(T\hat{W}) | \vec{\phi}_0, \vec{\psi}_0 \rangle = \int_{\vec{\phi}(0) = \vec{\phi}_0, \vec{\psi}(0) = \vec{\psi}_0}^{\vec{\phi}(T) = \vec{\phi}_T, \vec{\psi}(T) = \vec{\psi}_T} \mathcal{D}\vec{\phi}(t)\, \mathcal{D}\vec{\psi}(t) \exp(-\mathcal{S}[\{\vec{\phi}, \vec{\psi}\}]), \tag{8}$$

where the action reads

$$-\mathcal{S}[\{\vec{\phi}, \vec{\psi}\}] = -\int_0^T dt \left\{ \sum_{i=1}^N \phi_i(t) \frac{d\psi_i(t)}{dt} - \tilde{W}(\vec{\phi}(t), \vec{\psi}(t)) \right\}, \tag{9}$$

and the integral runs over all field configurations $\vec{\phi}(t), \vec{\psi}(t)$ over the time interval $t \in [0,T]$ matching the required boundary conditions at initial and final times.

Function $\tilde{W}$ encodes the action of the evolution operator $\hat{W}$ on the states. Its expression is obtained by first writing $\hat{W}$ in normal order form thanks to the (anti)commutation relations, then using the translation Table I, see Refs. [8,9,24]. For CP, we obtain $\tilde{W} = \tilde{W}_{\text{ann}} + \lambda \tilde{W}_{\text{cre}}$ with

$$\tilde{W}_{\text{ann}}(\vec{\phi}, \vec{\psi}) = \sum_{i=1}^N \phi_i [\exp(\psi_i) - 1],$$

$$\tilde{W}_{\rm cre}(\vec{\phi},\vec{\psi}) = \frac{1}{z}\sum_{i=1}^{N} \phi_i \sum_{j\in i} (1-\phi_j)[\exp(-\psi_j)-1]. \tag{10}$$

The previous quantum formalism allows us to express the expectation value of any observable of interest. For instance, we may start at time $t=0$ from a random state $|\rho_0\rangle$ with exactly $N_0=\rho_0 N$ occupied sites and project at the end on a state $\langle\rho_T|$ with exactly $N_T=\rho_T N$ occupied sites:

$$|\rho_0\rangle := \frac{1}{\binom{N}{N_0}} \sum_{\vec{s}} \otimes_{i=1}^{N}[(1-s_i)|0\rangle + s_i|1\rangle],$$

$$\langle\rho_T| := \sum_{\vec{s}} \otimes_{i=1}^{N}[(1-s_i)\langle 0| + s_i\langle 1|], \tag{11}$$

where the sums run over all states $\vec{s}$ with N_0 (N_T) occupation numbers s_i equal to 1, and the remaining $N-N_0$ ($N-N_T$) ones equal to 0. The probability that the density of particles equals ρ_T at time $t=T$ given that is was equal to ρ_0 at time $t=0$ is thus $P(\rho_T,T|\rho_0,0)=\langle\rho_T|\exp(T\hat{W})|\rho_0\rangle$. Using the path-integral formalism developed in this section, the logarithm Π of this probability reads

$$\Pi(\rho_T,T|\rho_0,0) = \ln\Bigg[\int \mathcal{D}\vec{\phi}(t)\,\mathcal{D}\vec{\psi}(t)\exp(-\mathcal{S}[\{\vec{\phi},\vec{\psi}\}]) \times\langle\rho_T|\vec{\phi}(T),\vec{\psi}(T)\rangle\langle\vec{\phi}(0),\vec{\psi}(0)|\rho_0\rangle\Bigg], \tag{12}$$

where the boundary conditions for the fields at initial and final times are now free. Knowledge of the above function gives access to the large deviations function defined in Eq. (1) through

$$\pi^*(\rho) = \lim_{T\to\infty}\lim_{N\to\infty}\frac{1}{N}\Pi(\rho,T|\rho^*,0). \tag{13}$$

Notice that, although there is no notion of energy nor Hamiltonian in CP, the form of its path-integral formulation closely looks like a classical mechanics Lagrangian, with a kinetic energy term and an effective potential energy term.

Calculation of the path integral on the right-hand side of Eq. (12) will be done through a perturbative expansion (in λ) of the effective potential for the average values of the fields $\vec{\phi}(t),\vec{\psi}(t)$, following an approach used in the context of classical statistical mechanics [29,30]. This expansion allows us to calculate quantities of interest, e.g., $\phi^*(\rho)$, λ_C, ρ^*, . . . , in powers of $1/D$. In the following, we will closely follow the technique and notations of Ref. [30] which makes use of this perturbation expansion scheme to calculate equilibrium properties of the Ising model in large dimensions. The main difference (and complication) is that, here, fields depend on time. An application of this approach to the study of the dynamics of continuous spins models can be found in Ref. [31].

B. Diagrammatic expansion of the effective potential

1. Constrained fields and conjugated sources

Let $\overline{\phi_i}(t)$ and $\overline{\psi_i}(t)$ be two arbitrary functions depending on time t and site i, with $\overline{\phi_i}\in[0,1]$, from which we define $\overline{\chi_i}(t) := [1-\overline{\phi_i}(t)]\{\exp[-\overline{\psi_i}(t)]-1\}$. We choose as elementary (site-attached) operators $\mathbb{1}-\hat{\phi}_i := \mathbb{1}-a_i^\dagger a_i$ and $\hat{\chi}_i := a_i^\dagger(\mathbb{1}+a_i)-\mathbb{1}$ [32], and impose the constraints

$$\langle\mathbb{1}-\hat{\phi}_i(t)\rangle = 1-\overline{\phi_i}(t), \quad \langle\hat{\chi}_i(t)\rangle = \overline{\chi_i}(t), \tag{14}$$

where

$$\langle\hat{A}\rangle = \frac{\langle\rho_T|\exp(\int_t^T dt'\,\hat{W})\,\hat{A}\,\exp(\int_0^t dt'\,\hat{W})|\rho_0\rangle}{\langle\rho_T|\exp(\int_0^T dt'\,\hat{W})|\rho_0\rangle}$$

is the average value of operator A at time t. This can be done through the introduction of Lagrange multipliers (sources) in the evolution operator: $\hat{W}$ is changed to $\hat{W}'(t)+W''(t)\mathbb{1}$ in the definition of $\langle\hat{A}\rangle$ where

$$\hat{W}'(t) := \mu\hat{W}_{\rm ann} + \lambda\hat{W}_{\rm cre} - \sum_i [h_i(t)(\mathbb{1}-\hat{\phi}_i) - g_i(t)\hat{\chi}_i],$$

$$W''(t) := \sum_i \{h_i(t)(1-\overline{\phi_i}(t)) - g_i(t)\overline{\chi_i}(t)\}. \tag{15}$$

Fields $h_i(t)$ and $g_i(t)$ are expected to be as regular as the imposed order parameters $\phi_i(t)$ and $\chi_i(t)$, and are assumed to be (at least) once differentiable with continuous derivatives over the time interval $t\in]0;T[$. However, to match with the components of the final bra and initial ket, Dirac's δ-singularities may be present at $t=0$ and $t=T$. Note the introduction of a new parameter μ in front of the annihilation operator in the expression of $\hat{W}'$. This parameter will result convenient for technical reasons only, and we will ultimately be interested in calculating quantities for $\mu=1$. This biased evolution operator allows us to express the logarithm of the probability that the final density equals ρ_T for a fixed set of order parameters,

$$\Pi[\rho_T,T;\{\overline{\phi},\overline{\chi}\}|\rho_0,0] = \ln\langle\rho_T|\hat{\mathcal{V}}(T,0)|\rho_0\rangle + \int_0^T dt\,W''(t), \tag{16}$$

and our task will be to compute $\hat{\mathcal{V}}(T,0) := \exp[\int_0^T dt\hat{W}'(t)]$. Requiring that Eq. (16) be extremal with respect to $\overline{\phi_i}(t)$ and $\overline{\chi_i}(t)$ in addition to the constraints above ensures that $h_i(t)=g_i(t)=0$ at the extremum of Π. Therefore, at the saddle point, Π in Eq. (16) will coincide with Π defined in Eq. (12).

The effective potential Π can be expanded in a double power series in λ, μ,

$$\Pi = \sum_{a,b\geq 0} \lambda^a\mu^b\Pi_{a,b} \quad \text{with} \quad \Pi_{a,b} := \frac{1}{a!}\frac{1}{b!}(\partial_\lambda)^a(\partial_\mu)^b\Pi|_{\lambda=\mu=0}. \tag{17}$$

We calculate below $\Pi_{0,0}$, that is, the effective potential in the absence of any evolution process albeit the one resulting

from the kinetic constraint over the order parameters, and then expose how to obtain higher orders in a,b through a systematic diagrammatic expansion. A nice feature of this expansion scheme is that, at any given order a in λ, we are able to resum the whole series in powers of μ and, thus, to express our result as a unique power series,

$$\Pi=\sum_{a\geqslant 0}\lambda^a\Pi_a(\mu) \quad \text{with} \quad \Pi_a:=\sum_{b\geqslant 0}\mu^b\Pi_{a,b}, \tag{18}$$

and set $\mu=1$ in the above expression.

2. Calculation of $\Pi_{0,0}$

We set $\lambda=0$. $\hat{W}'$ decouples into a tensor product over the sites. The latter remain however coupled by the constraints that the bra $\langle\rho_T|$ and the ket $|\rho_0\rangle$ correspond to configurations including exactly $N_T=\rho_T N$ and $N_0=\rho_0 N$ particles, respectively. We thus introduce two further Lagrange multipliers, ν_T and ν_0, to select the initial and final densities of particles. We replace $\langle\rho_T|$ and $|\rho_0\rangle$ in Eq. (16) with, respectively, $\langle\nu_T,\rho_T|:=\langle O|\exp[\nu_T\Sigma_i(\rho_T-a_i^\dagger a_i)]$ and $|\nu_0,\rho_0\rangle:=\binom{N}{N_0}^{-1}\exp[\nu_0\Sigma_i(a_i^\dagger a_i-\rho_0)]|O\rangle$, where $|O\rangle=(|0\rangle+|1\rangle)^{\otimes N}$ is the sum of all possible configurations. Note that $|\nu_0,\rho_0\rangle$ is normalized so as to represent a probability distribution. Once sites are decoupled, Π may be expressed as a sum of site-dependent effective potentials, each depending upon $\overline{\phi_i}(t)$, $\overline{\chi_i}(t)$, $h_i(t)$, $g_i(t)$, ν_T, and ν_0. We will eventually optimize the resulting Π over ν_T and ν_0 to ensure that the final and initial densities are the requested ones.

We send μ to zero to make $\hat{W}'$ diagonal in the basis $(|0\rangle,|1\rangle)$. This allows us to compute exactly the evolution operator $\hat{\mathcal{W}}(t_2,t_1):=\exp[\int_{t_1}^{t_2}\hat{W}'(t)dt]$, and then any average of operators or correlation function (CF), e.g., $\langle a_i(t_2)a_i^\dagger(t_1)\rangle:=\langle\nu_T,\rho_T|\hat{\mathcal{W}}(T,t_2)a_i\hat{\mathcal{W}}(t_2,t_1)a_i^\dagger\hat{\mathcal{W}}(t_1,0)|\nu_0,\rho_0\rangle$. Evaluating $\langle(\mathbb{1}-\hat{\phi}_i)(t)\rangle$ and $\langle\hat{\chi}_i\rangle$, and imposing constraints (14), we find back the rules listed in Table I with overbarred fields [33]. The expressions for the sources $h_i(t)$ and $g_i(t)$ are then [34], for times $0<t<T$,

$$h_i(t)=\frac{d}{dt}\overline{\psi_i}(t)+(e^{\overline{\psi_i}(t)}-1)\frac{d}{dt}\ln[1-\overline{\phi_i}(t)],$$

$$g_i(t)=-e^{\overline{\psi_i}(t)}\frac{d}{dt}\ln[1-\overline{\phi_i}(t)], \tag{19}$$

from which we obtain $h_i(t)[1-\overline{\phi_i}(t)]-g_i(t)\overline{\chi_i}(t)=[1-\overline{\phi_i}(t)]d/dt\,\overline{\psi_i}(t)$. In other words, the term in W'' of Eq. (16) gives back, aside boundary terms involving initial and final values, the "kinetic" term of the action $\mathcal{S}$ (9).

It appears that constraints (14) at times $t=0$ and $t=T$ can be imposed by nonsingular sources $h_i(t)$ and $g_i(t)$ only if the required state vectors $\langle\overline{\phi_i}(T),\overline{\psi_i}(T)|$ and $|\overline{\phi_i}(0),\overline{\psi_i}(0)\rangle$ are parallel to the initial bra $\langle\nu_T,\rho_T|$ and ket $|\nu_0,\rho_0\rangle$, respectively. To bypass this constraint, we introduce a singular term $h_{i,0}\delta(t-0)+h_{i,T}\delta(t-T)$ in the source $h_i(t)$—it is sufficient to modify $h_i(t)$ only and let $g_i(t)$ be regular, and we have also verified that singularities in $h_i(t)$ and $g_i(t)$ at times $t\in]0,T[$ are absent unless $\overline{\phi_i}(t)$ or $\overline{\psi_i}(t)$ are discontinuous, and that a discontinuity of the order parameters is not favorable in terms of action and can be discarded. Optimization of $\Pi_{0,0}$ with respect to $h_{i,0}$ and $h_{i,T}$ yields

$$h_{i,0}=\overline{\psi_i}(0)+\ln\left[\frac{\overline{\phi_i}(0)}{1-\overline{\phi_i}(0)}\right]-\nu_0, \quad h_{i,T}=\nu_T-\overline{\psi_i}(T), \tag{20}$$

and allows one to fulfill constraints (14) at initial and final times.

Gathering all contributions to $\Pi_{0,0}$ and using Stirling's formula, we find after some algebra

$$\begin{aligned}\Pi_{0,0}=\sum_i\Bigg[&\int_0^T dt\,\overline{\psi_i}(t)\frac{d\overline{\phi_i}(t)}{dt}+\nu_T[\rho_T-\overline{\phi_i}(T)]\\&-\nu_0[\rho_0-\overline{\phi_i}(0)]-\overline{\phi_i}(0)\ln\overline{\phi_i}(0)-[1-\overline{\phi_i}(0)]\\&\times\ln[1-\overline{\phi_i}(0)]\Bigg]+N[\rho_0\ln\rho_0+(1-\rho_0)\ln(1-\rho_0)].\end{aligned} \tag{21}$$

Notice that the sum of the last two terms in $\overline{\phi_i}(0)$ in Eq. (21) is equal to the entropy of N noninteracting particles at density $\overline{\phi_i}(0)$.

3. Perturbative expansions in powers of λ and μ

For the rest of this section, we call average of an operator $\hat{A}$, and denote by $\langle\hat{A}\rangle$, the ratio $\langle\nu_T,\rho_T|\hat{A}\hat{\mathcal{W}}(T,0)|\nu_0,\rho_0\rangle$ over $\langle\nu_T,\rho_T|\hat{\mathcal{W}}(T,0)|\nu_0,\rho_0\rangle$. Let us introduce the operators $\hat{S}_1=-\int_0^T dt\,\hat{W}_{\text{ann}}$ and $\hat{S}_2=-\int_0^T dt\,\hat{W}_{\text{cre}}$. These are directly related to Π through the relations $\partial_\mu\Pi=\langle-\hat{S}_1\rangle$ and $\partial_\lambda\Pi=\langle-\hat{S}_2\rangle$, valid for any λ and μ. The average values of the operators $\hat{S}_1$ and $\hat{S}_2$ are $\langle\hat{S}_1\rangle=-\int_0^T dt\,\Sigma_i\overline{\phi_i}(t)(\exp[\overline{\psi_i}(t)]-1)$ (for all λ, μ) and $\langle\hat{S}_2\rangle_{\lambda=0}=-\int_0^T dt\,\Sigma_i\overline{\phi_i}(t)\Sigma_{j\in i}\overline{\chi_j}(t)/z$ (only for $\lambda=0$), respectively, and give the beginning of the expansion of Π. The sequel is obtained by iterative application of the following identities true for any (differentiable) operator $\hat{A}$:

$$\partial_\mu\langle\hat{A}\rangle=\langle\partial_\mu\hat{A}\rangle+\langle\hat{A}\hat{U}\rangle, \quad \partial_\lambda\langle\hat{A}\rangle=\langle\partial_\lambda\hat{A}\rangle+\langle\hat{A}\hat{V}\rangle \tag{22}$$

with

$$\begin{aligned}\hat{U}=&-\hat{S}_1+\langle\hat{S}_1\rangle+\int_0^T dt\sum_i\,[\partial_\mu h_i(t)\{\hat{\phi}_i-\overline{\phi_i}(t)\}\\&+\partial_\mu g_i(t)\{\hat{\chi}_i-\overline{\chi_i}(t)\}],\end{aligned} \tag{23}$$

$$\begin{aligned}\hat{V}=&-\hat{S}_2+\langle\hat{S}_2\rangle+\int_0^T dt\sum_i\,[\partial_\lambda h_i(t)\{\hat{\phi}_i-\overline{\phi_i}(t)\}\\&+\partial_\lambda g_i(t)\{\hat{\chi}_i-\overline{\chi_i}(t)\}].\end{aligned} \tag{24}$$

Though sites are coupled by $\hat{V}$ through $\hat{S}_2$, successive applications of operators $\hat{U},\hat{V}$ permit to evaluate the (derivatives of) CFs required to compute the expansion in powers of μ and λ at $\lambda=0$ where these CFs are factorized over sites. Notice that $\hat{U}$, $\hat{V}$, and their derivatives with respect to μ and λ that will appear in higher orders of perturbation involve the derivatives of the fields h and g. These can be expressed in a convenient way from the identities $h_i(t) = -\partial_{\overline{\phi}_i(t)}\Pi$, $g_i(t) = -\partial_{\overline{\chi}_i(t)}\Pi$, $h_{i,T} = -\partial_{\overline{\phi}_i(T)}\Pi$ and $h_{i,0} = -\partial_{\overline{\phi}_i(0)}\Pi$. In particular, $\partial_\lambda h_{i,T} = \partial_{\overline{\phi}_i(T)}\langle\hat{S}_2\rangle = 0$ and $\partial_\lambda h_{i,0} = \partial_{\overline{\phi}_i(0)}\langle\hat{S}_2\rangle = 0$, allowing us to remove all terms involving δ's in h_i in the expressions of $\hat{U}$ and $\hat{V}$. Also, $\partial_\lambda h_i(t) = \partial_{\overline{\phi}_i(t)}\langle\hat{S}_2\rangle$ and $\partial_\lambda g_i(t) = \partial_{\overline{\chi}_i(t)}\langle\hat{S}_2\rangle$, so that the operator $\hat{V}$ writes in a convenient form when λ vanishes: $\hat{V}_{\lambda=0} = \int_0^T dt \Sigma_i \Sigma_{j\in i} \tilde{\phi}_i(t)\tilde{\chi}_j(t)/z$, where $\tilde{\phi}_i(t) = \hat{\phi}_i - \overline{\phi}_i(t)\mathbb{1}$ and $\tilde{\chi}_i(t) = \hat{\chi}_i - \overline{\chi}_i(t)\mathbb{1}$ express the deviations of the elementary operators with respect to their average values: $\langle\tilde{\phi}_i(t)\rangle = \langle\tilde{\chi}_i(t)\rangle = 0$ for all λ,μ. Finally, let us give some useful properties of $\hat{U}$ and $\hat{V}$.

(1) $\langle\hat{U}\rangle = \langle\hat{V}\rangle = 0$ (and if we write these operators in a natural way as sums over the graph sites, each summand $\langle\hat{U}_i\rangle$ and $\langle\hat{V}_i\rangle$ also vanishes).

(2) $\langle\hat{U}\tilde{\phi}_i(t)\rangle = \langle\hat{V}\tilde{\phi}_i(t)\rangle = \langle\hat{U}\tilde{\chi}_i(t)\rangle = \langle\hat{V}\tilde{\chi}_i(t)\rangle = 0$.

(3) Any CF of the type $\langle\hat{A}_1\hat{A}_2\cdots\hat{A}_k\hat{U}\rangle$ vanishes if the time attached to the $\hat{U}$ operator is smaller or larger than all other times attached to the $A_\not{}$ operators. Indeed, a direct evaluation of $\langle\nu_T,\rho_T|\hat{U}$ and $\hat{U}|\nu_0,\rho_0\rangle$ after explicitly expressing $\hat{U}$ in a similar way as we did for $\hat{V}_{\lambda=0}$ shows that both vectors vanish.

We now apply the above scheme to the calculation of Π.

III. MEAN-FIELD THEORY ($z\to\infty$ LIMIT)

In this section, we first expose the analysis of the contact process on a complete graph. We then explain how this mean-field theory can be found back through the formalism developed in Sec. II.

A. A simple derivation of mean-field theory: The contact process on the complete graph

Consider CP on the complete graph with N sites. As any two sites are adjacent, an exact account of the dynamics can be obtained from tracking the probability $p_n(t)$ that n sites are occupied at time t [35]. The master equation for these probabilities reads,

$$\frac{dp_n}{dt}(t) = (n+1)p_{n+1}(t) + \frac{\lambda}{N-1}(n-1)(N-n+1)p_{n-1}(t) - \left(n + \frac{\lambda}{N-1}n(N-n)\right)p_n(t), \tag{25}$$

with the conventions $p_{-1}(t) = p_{N+1}(t) = 0$. In the large N limit, we expect from the considerations of Sec. I B the following scaling behavior for the probabilities [36]:

$$p_n(t) = \exp[N\pi_{\rm MF}(n/N,t)]. \tag{26}$$

Inserting this scaling ansatz into the master equation (25) yields the equation of motion for the large deviation function $\pi_{MF}(\rho,t)$ of the density ρ of particles,

$$\partial_t\pi_{\rm MF}(\rho,t) = \tilde{W}_{MF}[\rho,\partial_\rho\pi_{\rm MF}(\rho,t)], \tag{27}$$

where

$$\tilde{W}_{\rm MF}[\phi,\psi] := \phi[\exp(\psi)-1] + \lambda\phi(1-\phi)[\exp(-\psi)-1]. \tag{28}$$

The very strong analogy between the above definition and the expression for the matrix elements of the creation and annihilation operators in Eq. (10) will be explained in the following section.

After a transient depending on the initial condition, e.g., all sites are initially occupied and all densities but $\rho=1$ have zero probability, the large deviation function $\pi_{\rm MF}$ relaxes to its stationary value,

$$\pi^*_{\rm MF}(\rho) = -\frac{1}{\lambda} + (1-\rho)[1-\ln\lambda-\ln(1-\rho)]. \tag{29}$$

It is maximal and equal to zero in $\rho=\rho^*$. The value in $\rho=0$ gives immediate access to the average lifetime of the metastable state with density ρ^*, that is, the time it takes to the system to reach the empty state, see Eq. (2),

$$t_{vac}(\lambda,N) \sim \exp\left[N\left(\frac{1}{\lambda}+\ln\lambda-1\right)\right]. \tag{30}$$

This value may be successfully compared to the results of Fig. 4 in Ref. [35]. A direct numerical simulation of the evolution of the $p_n(t)$ with N up to $\approx$100 has allowed us to check the validity of scaling hypothesis (26) and to obtain a perfect agreement of the experimental distribution with Eq. (29).

B. Mean-field theory from the "quantum" formalism

The first term $\Pi_{0,0}$ in the expansion of the effective potential Π in powers of λ and μ is given by Eq. (21). Then $\Pi_{1,0} = -\langle\hat{S}_1\rangle_{0,0}$ and $\Pi_{0,1} = -\langle\hat{S}_2\rangle_{0,0}$, the expressions of which in terms of $\overline{\phi}$ and $\overline{\chi}$ are given above. These are sufficient to establish the expressions of $\Pi_0(\mu)$ and $\Pi_1(\mu)$, due to the third property of Sec. II B 3. Indeed, we have the following.

(1) $\Pi_{a,0} = 0$ for all $a \geqslant 2$. *Proof:* $\partial_\mu\Pi = -\langle\hat{S}_1\hat{U}\rangle$ since $\partial_\mu\hat{S}_1 = 0$. The expression of $\langle\hat{S}_1\hat{U}\rangle$ involves a double sum over the sites, say, i,j, of terms of the form $\langle\hat{A}_i\hat{U}_j\rangle$. Any such CF vanishes for all μ as stated in Sec. II B 3.

(2) $\Pi_{a,1} = 0$ for all $a \geqslant 1$. *Proof:* $\partial_\mu\partial_\lambda\Pi = -\langle\hat{S}_2\hat{U}\rangle$ which, for $\lambda=0$ and all μ, reduces to a triple sum over the sites, say, i, $j\in i$ and k, of CF of the type $\langle\hat{A}_i\hat{B}_j\hat{U}_k\rangle$ where the times attached to $\hat{A}_i$ and $\hat{B}_j$ coincide. Again, these CF vanish due to the presence of the $\hat{U}$ operator.

As a result, setting $\mu=1$, we obtain

$$\Pi[\rho_T,T;\{\phi,\chi\}|\rho_0,0]$$
$$=\sum_i \Bigg[\nu_T[\rho_T-\overline{\phi}_i(T)]-\nu_0[\rho_0-\overline{\phi}_i(0)]$$
$$-\overline{\phi}_i(0)\ln[\overline{\phi}_i(0)]-[1-\overline{\phi}_i(0)]\ln[1-\overline{\phi}_i(0)]$$
$$+\rho_0\ln\rho_0+(1-\rho_0)\ln(1-\rho_0)+\int_0^T dt\Bigg(\overline{\psi}_i(t)\frac{d\overline{\phi}_i}{dt}(t)$$
$$+\overline{\phi}_i(t)\{\exp[\overline{\psi}_i(t)]-1\}+\frac{\lambda}{z}\overline{\phi}_i(t)\sum_{j\in i}\overline{\chi}_j(t)\Bigg)\Bigg]$$
$$+O(\lambda^2). \tag{31}$$

For $\lambda=0$ (for $\mu=0$), we are able to compute action (31) directly, without using such a perturbative expansion as Eq. (17), since the matrix of $\hat{W}'$ is upper (lower) triangular in the basis $(|0\rangle,|1\rangle)$. However, when both λ and μ are nonzero, we do not know how to proceed without the perturbative expansion.

In search for a translationally invariant, i.e., site-independent evolution, we choose all quantities to be site independent and remove site indices. We also drop the bars over the fields to simplify notations. Equation (31) then becomes $\pi_{\rm MF}=\Pi/N$ with

$$\pi_{\rm MF}[\rho_T,T;\{\phi,\chi\}|\rho_0,0]$$
$$=-\phi(0)\ln[\phi(0)]-[1-\phi(0)]\ln[1-\phi(0)]+\rho_0\ln\rho_0$$
$$+(1-\rho_0)\ln(1-\rho_0)+\nu_T[\rho_T-\phi(T)]-\nu_0[\rho_0-\phi(0)]$$
$$+\int_0^T dt\Bigg(\psi(t)\frac{d\phi}{dt}(t)+\tilde{W}_{\rm MF}[\phi(t),\psi(t)]\Bigg), \tag{32}$$

where $\tilde{W}_{\rm MF}$ is defined in Eq. (28). The above expression suffices to the study the mean-field (MF) case, i.e., when the site connectivity z goes to infinity. This may happen for large complete graphs, where each site is connected to all other sites $(z=N-1)$, or in the $D\to\infty$ limit of a D-dimensional regular lattice $(z=2D)$. As shown in Sec. IV A, higher-order terms in the λ expansion give $O(1/z)$ additive contributions to Π (within a site-independent ansatz), and vanish in the $z\to\infty$ limit. Therefore, $\pi_{\rm MF}$ is the exact mean-field expression for the action. To obtain the (exponentially in N) dominant trajectory of the order parameters $\phi(t),\psi(t)$, we first extremize Eq. (32) with respect to ν_T,ν_0, to get the expected relations $\phi(T)=\rho_T$ and $\phi(0)=\rho_0$. Notice that, if the initial state were a superposition of configurations with various densities, e.g., $\int_0^1 d\rho_0\exp[Nq(\rho_0)]|\rho_0\rangle$, Eq. (32) would include an additive contribution $q(\rho_0)$; the most probable initial density ρ_0 would then be given by the solution of $\partial_\rho q(\rho_0)=\psi(0)$. The resulting expression,

$$\pi_{\rm MF}=\int_0^T dt\Bigg\{\psi(t)\frac{d\phi}{dt}(t)+\tilde{W}_{\rm MF}[\phi(t),\psi(t)]\Bigg\} \tag{33}$$

has then to be functionally extremized over the fields $\phi(t)$ and $\psi(t)$. The equations of motion (EM) for the fields are the Hamilton-Jacobi equations associated to Lagrangian (33),

$$\frac{d\psi}{dt}(t)=\partial_\phi\tilde{W}_{\rm MF}[\phi(t),\psi(t)],$$
$$\frac{d\phi}{dt}(t)=-\partial_\psi\tilde{W}_{\rm MF}[\phi(t),\psi(t)] \tag{34}$$

along with the already established initial and final conditions: $\phi(T)=\rho_T$ and $\phi(0)=\rho_0$.

The solution of the EM yields the logarithm $N\pi_{\rm MF}$ of the probability to go from a configuration with density $\phi(0)$ at time 0 to another configuration with density $\phi(T)$ at time T. To solve these equations, we make use of the fact that $\tilde{W}_{\rm MF}$ is a conserved quantity from Eq. (34), which we denote by E. Then, the density ϕ and the time t can be expressed as functions of $y:=\exp(\psi)$,

$$t=\int_{y(0)}^{y} dy'[(y'-\lambda)^2(y'-1)^2+4E\lambda y'(y'-1)]^{-1/2}. \tag{35}$$

The action of the trajectory equals the large deviation function, $\pi_{\rm MF}(\rho,T)=\int_{y(0)}^{y(T)}dy'\ln(y')\partial_y\phi(y')+TE$. The shape of the solutions of Eq. (34) depends on the sign of $\psi(0)$. As shown in Fig. 3, if we exclude solutions where $\phi(t)$ is always zero [37], three cases have to be distinguished.

(1) If $\psi(0)=0$, the solutions have an infinite lifetime. $\psi(t)$ remains zero at all times [38], and the field $\phi(t)$ obeys the first-order ordinary differential equation

$$\frac{d\phi}{dt}(t)=-\lambda\phi(t)\Bigg(\phi(t)-1+\frac{1}{\lambda}\Bigg). \tag{36}$$

This equation coincides with the mean-field equation for the density $\rho(t)$, straightforwardly obtained when neglecting correlations between occupation numbers of neighboring sites. At large times, $\phi(t)$ tends to 0 or $\rho^*=1-1/\lambda$ depending on whether λ is smaller or larger than the critical value $\lambda_C=1$ as shown in Fig. 1(a). Notice that the action $\pi_{\rm MF}$ vanishes as $\psi=0$.

(2) If $\psi(0)<0$, the solutions have a finite lifetime and $\phi(t)\to 1$ while $\psi(t)\to-\infty$ [see Figs. 3(a,b)].

(3) If $\psi(0)>0$, the sign of the conserved quantity E matters. If $E>0$ (which is necessary if $\lambda<1$), the lifetime is finite [see Fig. 3(c)]. If $E<0$, the solutions are periodic [see Fig. 3(d)]. If $E=0$, the situation is the natural intermediate between the two cases. In all cases, the lifetime (or the period) $T(E)$ increases as $|E|$ diminishes.

Nonzero fields ψ select instantonic solutions allowing the system to escape the typical behavior described by the $\psi=0$ solution. These solutions have an extensive action, and are therefore exponentially suppressed when the system size increases. However, they are the solutions giving rise to large deviations of the density for a finite volume [Fig. 1(b)]. The most probable fluctuations correspond to long times solutions, i.e., $E\to 0$. In this case, $T(E)$ diverges like $\log E$, and

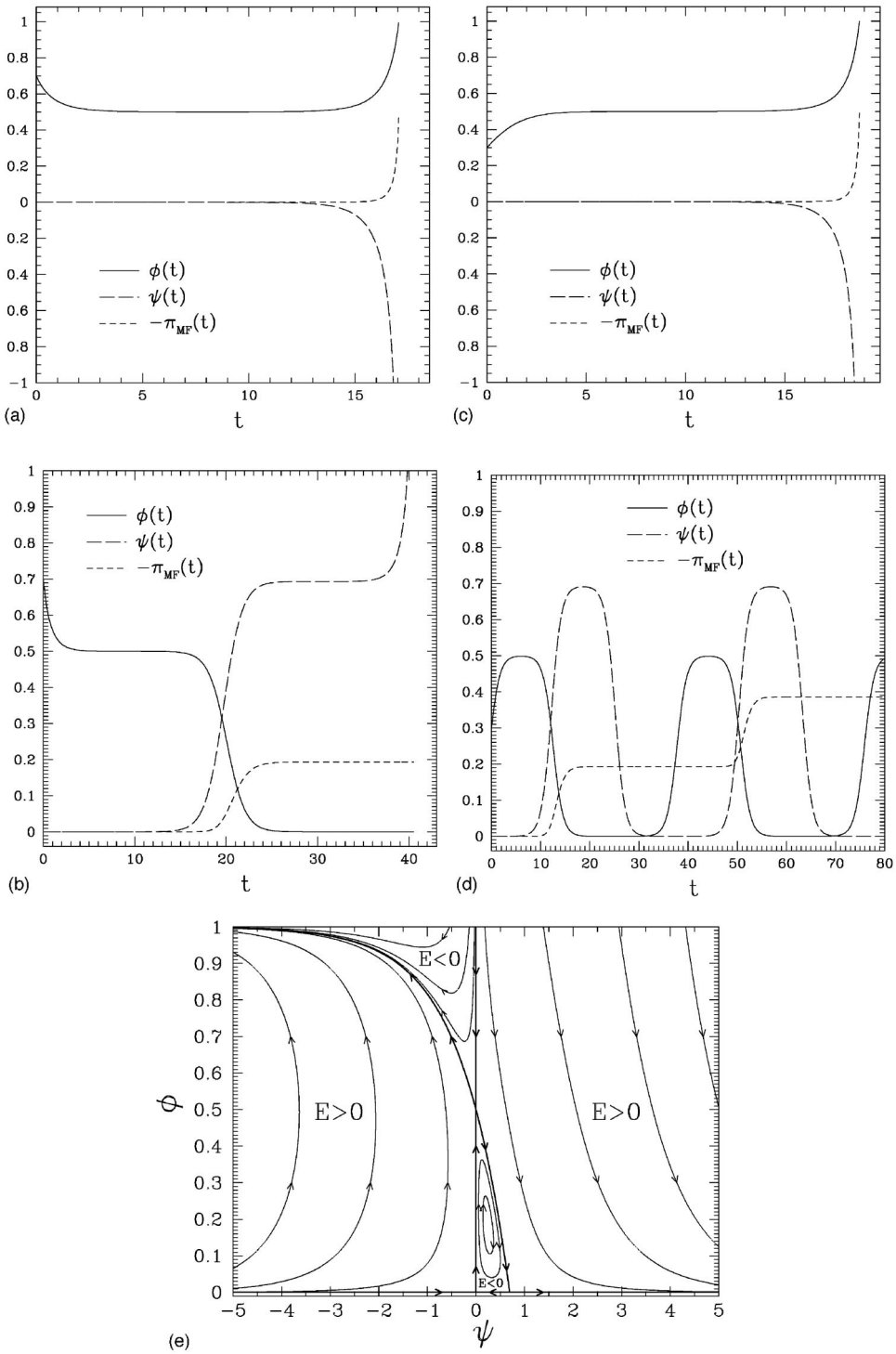

FIG. 3. Solutions of the mean-field equations of motion (34) for $\lambda=2$ ($\rho^*=1/2$) (A and B). For negative $\psi(0)$ ($=-10^{-7}$ here), the solutions have a finite lifetime. After quickly reaching the most probable value of the density of particles, ρ^*, $\phi(t)$ stays for a long time in the neighborhood of ρ^* but finally reaches unity, while $\psi(t)\to-\infty$. The action π_{MF} tends to a negative finite value; the main contribution to it comes from the final jump of ϕ from ρ^* to 1. (C) For positive $\psi(0)$ ($=10^{-8}$ here) and $E>0$, the lifetime is finite. After quickly reaching ρ^*, $\phi(t)$ stays for a long time in its neighborhood but finally transits to the neighborhood of 0 where it stays again for a long time, while $\psi(t)$ transits to $\ln\lambda$ and stays close to it. Finally $\psi(t)\to+\infty$ while $\phi(t)\to0$. π_{MF} tends to a negative finite value, the main contribution of which is accumulated during the transit. (D) For positive $\psi(0)>0$ ($=10^{-8}$ here) and $E<0$, the solution is periodic. $\phi(t)$ and $\psi(t)$ oscillate between two values inside the $[0,\rho^*]$ and $[0,\ln(\lambda)]$ intervals, respectively, and the action diverges to $-\infty$ by hops. (E) Phase portrait with all types of solutions (oriented according to the time evolution). The phase space divides into four regions delimited by the solutions for which $E=0$ (represented in thick lines); in each region the sign of E is indicated. The quasistationary state appears on this diagram as the crossing point ($\psi=0,\phi=\rho^*$) of two solutions with $E=0$: it is stable along the ϕ direction but instable along the ψ direction.

the *TE* term vanishes. When $\lambda>1$, we have the simple identity $\phi(y)=1-y/\lambda$ if $0\leqslant y\leqslant\lambda$, 0 if $y\geqslant\lambda$. In particular, the weight of the instantonic solution that goes from $\phi(0)=\rho^*$ to $\phi(+\infty)=\rho$ coincides with the stationary large deviation function for the density $\pi^*_{\mathrm{MF}}(\rho)$ defined in Eq. (29).

The large deviation function can be obtained at any finite time t too. To do so, we use expression (32) to express the probability of going from the state with distribution $\pi(\rho,t)$ at time t to the one the state with $\pi(\rho,t+dt)$ at time $t+dt$. Special care must be paid to discretizing the term involving time derivations in a symmetric way between t and $t+dt$ as requested for path integrals [28]. The resulting evolution equation for the large deviation function coincides with Eq. (27) as expected.

C. Relationship with Martin-Siggia-Rose and Janssen–de Dominicis formalisms

The above formalism is, to some extent, related to the treatment of Langevin equations by Martin, Siggia, and Rose (MSR) [39] and Janssen and de Dominicis [40–42]. If $x(t)$ is a classical (scalar or vector) field, the Langevin equation

$$\frac{dx}{dt}(t)=-V'(x(t))+\eta(t) \tag{37}$$

describes its evolution in the potential V (V' denotes $\partial_x V$) under the random Gaussian force η. η is specified by its first two moments: $\overline{\eta(t)}=0$, $\overline{\eta(t)\,\eta(t')}=2T\delta(t-t')$, where T is the temperature and the overbars denote the noise average. Let $P(x_T,T|x_0,0)$ be the probability that x equals x_T at time T conditioned to its initial value. This probability can be expressed as a path integral through the introduction of a response variable $\hat{x}$ conjugated to x [39–42],

$$P(x_T,T|x_0,0)=\int_{x(0)=x_0}^{x(T)=x_T}\mathcal{D}x(\tau)\mathcal{D}\hat{x}(\tau)\exp\left[\int_0^t d\tau\left\{i\hat{x}(\tau)\times\left(\frac{dx}{dt}(\tau)+V'(x(\tau))\right)-T\hat{x}^2(\tau)\right\}\right]. \tag{38}$$

Functional optimization of Eq. (38) with respect to $x,\hat{x}$ yields the classical equations of motion,

$$\frac{dx(t)}{dt}=-V'(x(t))-i2T\hat{x}(t),\quad \frac{d\hat{x}(t)}{dt}=\hat{x}(t)V''(x(t)) \tag{39}$$

from which we obtain that $dx/dt(t)^2-V'(x(t))^2$ is a constant of motion.

These EMs are formally identical to those derived for CP (34) in Sec. III (x playing the role of ϕ and $\hat{x}$ that of $-i\psi$) when $|\psi|\ll 1$, with the following choice of potential and temperature:

$$V'(\phi)=\lambda\phi(\phi-\phi^*),\quad 2T(\phi)=\phi(1+\lambda(1-\phi)). \tag{40}$$

Therefore, in the weakly fluctuating regime where ψ is small and ϕ close to its most probable value ρ^*, the system evolves in an effective potential V with fluctuations that can be described by a Langevin equation at temperature T [43]. This description breaks down as soon as we consider large deviations, or transitions from the metastable to the empty state, as can be seen from the numerical comparison of the true solutions of Eq. (34) with the solutions of Eq. (39).

Extending the validity of the Langevin equation approach to the full domain of ϕ and ψ would require the use of a MSR-like formalism [39–42]. Interestingly, MSR stated in their original work that the knowledge of the physical field ϕ alone is not sufficient to compute all quantities of interest beyond the Gaussian approximation, and that the introduction of a second operator (corresponding to our ψ, or to a and $a^\dagger$, whereas ϕ corresponds to $a^\dagger a$) to express the response functions of the physical field was required.

IV. FINITE-DIMENSION THEORY (1/z EXPANSION)

A. Analytical calculation

Calculation of the corrections to mean-field theory requires the knowledge of higher-order terms in the expansion of Π in powers of λ and μ. Strictly speaking, our expansion is, after we resum the μ-expansion, an expansion in powers of λ, or, more precisely, of λ/z. It naturally gives access to an expansion of Π in powers of $1/z$ as shown below.

1. The diagrammatic expansion

To show how this expansion works in practice, let us consider the first correction to Eq. (32), $2\,\Pi_{2,0}=\partial_\lambda^2\Pi|_{0,0}=-\partial_\lambda\langle\hat{S}_2\rangle_{0,0}=-\langle\hat{S}_2\hat{V}\rangle_{0,0}=\langle\hat{V}^2\rangle_{0,0}$ since $\partial_\lambda\hat{S}_2=0$ and $\langle\hat{S}_2\hat{V}\rangle=-\langle\hat{V}^2\rangle$. $\hat{V}_{0,0}$ involves a sum over couples of neighboring sites that can be written as a sum over oriented links. The term $\tilde{\phi}_i\tilde{\chi}_j$ will be represented by a link going from site i to site j. Therefore $\langle\hat{V}^2\rangle_{0,0}$ writes as a sum over couples of oriented links. When $\lambda=0$, sites decouple and terms where a site carries a single operator $\tilde{\phi}$ or $\tilde{\chi}$ vanish (Sec. II B 3). We are thus left with terms where two parallel links loop over two neighboring sites i,j on the lattice,

$$i\leftrightarrows j=\int_0^T \mathrm{d}t\int_0^T \mathrm{d}t'\,\langle\tilde{\phi}_i(t)\,\tilde{\chi}_j(t)\,\tilde{\phi}_i(t')\,\tilde{\chi}_j(t')\rangle_{0,0}\,, \tag{41}$$

and terms with the same structure but links pointing in opposite directions. As $\lambda=0$, this four-point CF factorizes into a product of two two-point CFs:

$$\langle\tilde{\phi}_i(t)\tilde{\chi}_j(t)\tilde{\phi}_i(t')\tilde{\chi}_j(t')\rangle_{0,0}=\langle\tilde{\phi}_i(t)\tilde{\phi}_i(t')\rangle_{0,0}\langle\tilde{\chi}_j(t)\tilde{\chi}_j(t')\rangle_{0,0}.$$

Each of these CFs can be straightforwardly computed, e.g., $\langle\tilde{\phi}_i(t)\tilde{\phi}_i(t')\rangle_{0,0}=\overline{\phi_i}(t_1)[1-\overline{\phi_i}(t_2)]$ where $t_1=\min(t,t')$ and $t_2=\max(t,t')$. The final result reads

$$i \leftrightarrows j = -2 \int_0^T \mathrm{d}t_2 \int_0^{t_2} \mathrm{d}t_1 \, \overline{\phi}_i(t_1) \left(1 - \overline{\phi}_i(t_2)\right) \left(1 + \overline{\chi}_j(t_1)\right) \overline{\chi}_j(t_2) \,. \tag{42}$$

The antiparallel two-site loop diagram may be evaluated in the same way. Notice that the final outcome does not depend on the indices i,j of the sites, provided these are neighbors on the lattice. We will therefore drop site indices in the following. Then, we count the multiplicity of each diagram, equal to Nz for both parallel and antiparallel two-sites loops. Finally, each diagram gets a factor $1/z^2$ coming from the $(\lambda/z)^2$ factor in $\hat{W}_{\mathrm{cre}}$. As a result, the net contribution will be of the order of $1/z$, that is, $1/D$ on a D-dimensional hypercubic lattice.

We are now able to write the general expression of the $1/z$ expansion in a graphical way. For instance, for a hypercubic lattice of dimension D (and site connectivity $z=2D$),

$$\pi = \pi_{\mathrm{MF}} + \frac{\lambda^2}{2!(2D)^2} D \leftrightarrows + \frac{\lambda^3}{3!(2D)^3} D \leftrightarrows + \frac{\lambda^4}{4!(2D)^4} D(2D-1)6 \leftrightarrows + \frac{\lambda^4}{4!(2D)^4} \frac{D(D-1)}{2} 4! \square + \frac{\lambda^4}{4!(2D)^4} D \leftrightarrows + \cdots \,. \tag{43}$$

Each undirected diagram in the above expansion represents the sum of the correlation functions (like the one entering $\Pi_{2,0}$ and evaluated above) that share the same support on the graph but differ by the orientations of the links. There are 2^ℓ link orientations for an undirected diagram with ℓ links. The coefficients in front of the diagrams take into account the power of λ/z (equal to the number of links in the diagram), the inverse factorial from the Taylor formula, and a combinatorial factor. This combinatorial coefficient is the product of the multiplicity of the undirected diagram (number of times it can be drawn on the lattice, divided by the lattice size N) and of the number of ways to associate a time t to each link of the diagram when evaluating the CF [44]. As one may infer from the first diagrams, there is only a finite number of terms contributing to a given order in $1/z$.

2. Summation of the μ-expansion and memory kernels

Π being the logarithm of a generating function of the fields, all the diagrams entering expansion (43) are connected. Moreover, for $\mu=0$ all nonirreducible diagrams, i.e., which may be cut into two, or more, pieces by removal of a vertex vanish, as in the virial expansion [45] and possibly the Ising model [30]. This statement does unfortunately not extend to nonzero μ. To get the μ-expansion we make repeated uses of the leftmost identity in Eq. (22). As $\partial_\mu \hat{U} = \partial_\mu \hat{V} = 0$, this amounts to insert $\hat{U}$ operators (one for each power of μ) in the CFs, yielding contributions of the form

$$D_n := \int_0^T dt_1 \int_0^T dt_2 \cdots \int_0^T dt_{n+2} \langle \tilde{\phi}_i(t_1) \times \hat{U}_i(t_2) \hat{U}_i(t_3) \cdots \hat{U}_i(t_{n+1}) \tilde{\phi}_i(t_{n+2}) \rangle . \tag{44}$$

As stated in Sec. II B 3, such a term vanishes if one of the times $t_2, t_3, \ldots, t_{n+1}$ associated to the $\hat{U}$ operators is the minimum or maximum of all times. If not, the integrand is the product of factors

$$\overline{\xi}(t_k) := -\frac{\exp \overline{\psi}(t_k)}{1 - \overline{\phi}(t_k)} \tag{45}$$

for each $\hat{U}(t_k)$ and a factor depending on the other operators involved in the CF. If there are strictly less than four other operators in the CF or no $\hat{U}$ operator between the second and the second last times, this latter factor is equal to the CF where all $\hat{U}$ have been removed; for instance, the term D_n defined in Eq. (44) reads

$$D_n = 2 \int_0^T dt \int_0^t dt' \langle \tilde{\phi}_i(t) \tilde{\phi}_i(t') \rangle \left(\int_{t'}^t dt'' \overline{\xi}_i(t'') \right)^n . \tag{46}$$

If the original CF involves more operators or a "badly" located $\hat{U}$, there appears a kind of disentanglement of the original operators. Consider, for instance, the four-field CF $D' := \langle \tilde{\phi}_i(t_1) \tilde{\phi}_i(t_2) \tilde{\phi}_i(t_3) \tilde{\phi}_i(t_4) \rangle$ with $t_1 < t_2 < t_3 < t_4$. A direct evaluation shows that D' equals $-\overline{\phi}_i(t_1)[-1 + \overline{\phi}_i(t_4)][-\overline{\phi}_i(t_3) + 1 + 3\overline{\phi}_i(t_2)\overline{\phi}_i(t_3) - 2\overline{\phi}_i(t_2)]$ and cannot be expressed as a product of four factors, each of which would be associated to a time t_j. We shall say that D' is entangled, here due to the t_2, t_3 term. Insertion of at least one $\hat{U}_i$ between t_2 and t_3, as in

$$D'' := \langle \tilde{\phi}_i(t_1) \hat{U}_i(t'_1) \hat{U}_i(t'_2) \cdots \hat{U}_i(t'_{n_1}) \tilde{\phi}_i(t_2) \hat{U}_i(t'_{n_1+1}) \times \hat{U}_i(t'_{n_1+2}) \cdots \hat{U}_i(t'_{n_2}) \tilde{\phi}_i(t_3) \hat{U}_i(t'_{n_2+1}) \times \hat{U}_i(t'_{n_2+2}) \cdots \hat{U}_i(t'_{n_3}) \tilde{\phi}_i(t_4) \rangle$$

with

$t_1<t_1'<\cdots<t_{n_1}'<t_2<t_{n_1+1}'<\cdots<t_{n_2}'<t_3<t_{n_2+1}'<\cdots<t_{n_3}'<t_4$ removes this entanglement. D'' is the product of factors $\overline{\xi_i}(t_k')$, one for each $\hat{U}(t_k')$, and of the disentangled (factorized) expression $-\overline{\phi_i}(t_1)[-1+\overline{\phi_i}(t_4)][-1+2\overline{\phi_i}(t_2)][-1+2\overline{\phi_i}(t_3)]$. We conclude that a CF of the type

$$D_n'' \coloneqq \int_0^T dt_4 \int_0^T dt_3 \int_0^T dt_2 \int_0^T dt_1 \int_0^T dt_1' \int_0^T dt_2' \cdots \int_0^T dt_n' \times \langle \tilde{\phi}_i(t_1)\tilde{\phi}_i(t_2)\tilde{\phi}_i(t_3)\tilde{\phi}_i(t_4)\hat{U}_i(t_1')\hat{U}_i(t_2')\cdots\hat{U}_i(t_n')\rangle \tag{47}$$

can be expressed as

$$\begin{aligned} D_n'' = {} & 24\int_0^T dt_4 \int_0^{t_4} dt_3 \int_0^{t_3} dt_2 \int_0^{t_2} dt_1 \langle \tilde{\phi}_i(t_1)\tilde{\phi}_i(t_2) \\ & \times \tilde{\phi}_i(t_3)\tilde{\phi}_i(t_4)\rangle_{\mathrm{dis}} \left(\int_{t_1}^{t_4} dt \overline{\xi_i}(t) \right)^n \\ & + 24\int_0^T dt_4 \int_0^{t_4} dt_3 \int_0^{t_3} dt_2 \int_0^{t_2} dt_1 \\ & \times [\langle \tilde{\phi}_i(t_1)\tilde{\phi}_i(t_2)\tilde{\phi}_i(t_3)\tilde{\phi}_i(t_4)\rangle \\ & - \langle \tilde{\phi}_i(t_1)\tilde{\phi}_i(t_2)\tilde{\phi}_i(t_3)\tilde{\phi}_i(t_4)\rangle_{\mathrm{dis}}] \\ & \times \left(\int_{t_1}^{t_2} dt \overline{\xi_i}(t) + \int_{t_3}^{t_4} dt \overline{\xi_i}(t) \right)^n, \end{aligned} \tag{48}$$

where the ''dis'' subscript means that the disentangled expression for the CF integrand $\langle \cdots \rangle$ must be taken.

It appears that, at any given order in λ, the series expansion in powers of μ can be easily summed up, yielding memory kernels in the resulting $\Pi_a(\mu)$ with $a \geqslant 2$. For instance, $\int_0^T dt \int_0^T dt' \langle \tilde{\phi}_i(t)\tilde{\phi}_i(t')\rangle$ is replaced with

$$\sum_{n\geqslant 2} \frac{\mu^n}{n!} D_n = \int_0^T dt \int_0^T dt' \langle \tilde{\phi}_i(t)\tilde{\phi}_i(t')\rangle \times \exp\left(\mu \int_{\min(t,t')}^{\max(t,t')} dt'' \overline{\xi_i}(t'') \right), \tag{49}$$

the memory kernel being the exponential term, where μ is eventually set to 1. Due to the presence of the kernel, the CF between two operators at times t and t' decreases with a time difference $|t-t'|$ (remember $\overline{\xi}<0$).

This property extends to more than two operators. The contribution of a diagram with n links, thus of order λ^n in the λ-expansion of Π, may be written as the sum of a finite number of terms of the form

$$F \coloneqq \int_0^T dt_n \int_0^{t_n} dt_{n-1} \cdots \int_0^{t_2} dt_1 P \times \exp\left(i_1 \int_{t_1}^{t_2} dt \overline{\xi}(t) + \cdots + i_n \int_{t_{n-1}}^{t_n} dt \overline{\xi}(t) \right), \tag{50}$$

where P is a polynomial in $\phi(t_1)$, $\exp[-\psi(t_1)], \ldots, \phi(t_n)$ and $\exp[-\psi(t_n)]$ and $i_1, i_2, \ldots, i_n$ are positive integers. The presence of the memory kernels ensures that the integrand sharply decreases as $t_n - t_1$ increases.

One may wonder why memory kernels appear in the expressions above, whereas CP is a Markovian stochastic process. This is the consequence of the projection of the complete distribution of states, $|P(t)\rangle$, that is, the knowledge of the probability of occupation or vacancy of all sites, onto a partial description where we keep track of the order parameters $\phi(t), \psi(t)$ only. Beyond mean field, the degrees of freedom which were discarded pop up as non-Markovian contributions to the dynamical evolution of the order parameters. This phenomenon is well known, and can be illustrated with an elementary example proposed in the Appendix.

B. Results and comparison with simulations

Following the above recipes, the effective potential π may be expanded in powers of $1/z$, see Eq. (43). The explicit expression for the first correction to mean field, coming from the two-site loop diagram, reads

$$\pi_1 = -\frac{2\lambda^2}{z} \int_0^T dt_2 [1-\phi(t_2)]^2 (e^{-\psi(t_2)}-1) \int_0^{t_2} dt_1 \phi(t_1) \times \{[1-\phi(t_1)]e^{-\psi(t_1)} + \phi(t_1)\} \exp\left(2\int_{t_1}^{t_2} dt'' \xi(t'') \right). \tag{51}$$

The $O(1/z^2)$ corrections to π required the calculation of the diagrams listed in Eq. (43). The resulting expression, π_2, for the D-dimensional hypercubic lattice (where $z=2D$) is too lengthy to be given here, but can be obtained with the help of a computer algebra software. This gives, as a by-product, the expression π_2 for the Cayley lattice (infinite graph without loops where all sites have exactly z neighbors) after removal of the square diagram ${}_l^i\square_k^j$.

Functional optimization of the resulting expression for π with respect to $\phi(t)$ and $\psi(t)$ yields EMs which include corrections of orders $1/z$ and $1/z^2$ to the Hamilton-Jacobi equations (34). These corrections involve terms with multiple integrals on the time.

1. Corrections to the density ρ^* of particles and the critical parameter λ_C

We first concentrate on the solution to the EM with vanishing $\psi(t)$ at all times t. The equation for $\phi(t)$ then simplifies; for instance, to the first order in $1/z$, we obtain

$$\frac{d\phi}{dt}(t) = -\lambda\phi(t)\left(\phi(t) - 1 + \frac{1}{\lambda}\right) - \frac{2\lambda^2}{z}[1-\phi(t)]^2 \times \int_0^t dt'\,\phi(t')\exp\left(-2\int_{t'}^t \frac{dt''}{1-\phi(t'')}\right). \quad (52)$$

With the help of computer algebra, the EM for $\phi(t)$ can be written up to order $1/z^2$, and its asymptotic behavior analyzed. We find that $\phi(t\to\infty)$ equals 0 or $\rho^*>0$ depending on the value of the parameter λ with respect to its critical value λ_C. The asymptotic density reads

$$\rho^* = 1 - \frac{1}{\lambda} - \frac{1}{\lambda^2 z} - \frac{6\lambda^2+11\lambda+3}{6\lambda^4 z^2} + O(1/z^3) \quad (53)$$

on the D-dimensional hypercubic lattice ($z=2D$), and

$$\rho^* = 1 - \frac{1}{\lambda} - \frac{1}{\lambda^2 z} - \frac{6\lambda^2+11\lambda-3}{6\lambda^4 z^2} + O(1/z^3) \quad (54)$$

on the Cayley tree where all sites have z neighbors. The critical value λ_C can be easily obtained from the above equations as the value of the parameter λ below which no state with a finite density of particles can survive. This is intended to be the lower critical value $\lambda_{C_{\text{lower}}}$ on the Cayley tree [13(b)], where there exists an intermediate range $[\lambda_{C_{\text{lower}}}, \lambda_{C_{\text{upper}}}]$ of values of λ where nonuniform metastable states can survive without invading the whole graph while, above $\lambda_{C_{\text{upper}}}$, there is a single uniform metastable state—on hypercubic lattices, both thresholds coincide. Setting $\rho^*=0$, we obtain

$$\lambda_C = 1 + \frac{1}{z} + \frac{7}{3z^2} + O(1/z^3) \quad (55)$$

on a the hypercubic lattice, and

$$\lambda_C = 1 + \frac{1}{z} + \frac{4}{3z^2} + O(1/z^3) \quad (56)$$

on the Cayley tree. These results are compatible with the rigorous bounds $[1-1/(2D)]^{-1} \leqslant \lambda_C \leqslant 4$ (hypercubic lattice) and $1 \leqslant \lambda_C \leqslant (1-2/z)^{-1}$ (on the Cayley tree) [13]. Notice that the lower bound $\lambda_C \geqslant [1-1/(2D)]^{-1}$ was obtained [13(a)] through a two-site calculation. When discarding all diagrams but the two-site loops, we find $\lambda_C = 1 + 1/(2D) + 1/(2D)^2 + O(1/(2D)^3)$, that is, the same bound. For small dimensions, our asymptotic results are of poor quality. We refer the interested reader to the various works that give more precise estimates for λ_C, e.g., for hypercubic lattices in $1 \leqslant D \leqslant 5$ Ref. [46], for $D=1$ through series expansions Refs. [47,48].

Our values of ρ^* are in good agreement with numerical simulations carried out on hypercubic lattices in dimensions up to $D=10$ for several values of $\lambda(=1.5,2,3)$. Simulating large size lattices in higher dimensions would require prohibitive memory space. Instead, we have performed simulations of the conserved contact process (CCP) [49]. This is a canonical counterpart of CP where the number of occupied sites is kept constant, but λ fluctuates. The stationary properties of both processes are, in the limit of infinite lattice size, equivalent [50,51]. In particular, simulating CCP with a (not too large) number N of particles on an almost infinite lattice (in our simulation, of size $L=2^{32}$) amounts to simulate CP with a vanishing density. The average value of λ in CCP then coincides with the critical λ_C in CP. We have been able to simulate CCP on hypercubic lattices with up to $N=4000$ sites and in dimensions up to $D=80$ or up to $z=81$ on the Cayley tree [52]. Results are displayed in Fig. 4, and are in very good agreement with our theoretical predictions for λ_C, Eqs. (55), (56), and previous simulations [46].

2. Corrections to the distribution of particle densities

The analytical resolution of the EM when $\psi(t)\neq 0$ is difficult. We have restricted ourselves to a first order in $1/z$ expansion around the infinite lifetime solutions for which we have an analytical expression in the mean-field case. It is convenient to parametrize the real time t in terms of y_0 introduced in Eq. (35): $y_0 = \exp[\psi_0(t)]$, where $\psi_0(t)$ is the mean-field expression for $\psi(t)$. In the thermodynamic limit $N\to\infty$ with $E\to 0$ (infinite lifetime), the $t\to+\infty$ limit translates into the $y_0\to\lambda$ limit.

In this setting, we may write $\phi(y_0) = \phi_0(y_0) + \phi_1(y_0)/z + O(1/z^2)$ and similarly $\psi(y_0) = \psi_0(y_0) + \psi_1(y_0)/z + O(1/z^2)$, where ϕ_0 and ψ_0 were computed previously for the mean-field case. From the EM, we derive two coupled first-order linear differential equations for ϕ_1 and ψ_1:

$$(y_0-1)(\lambda-y_0)\frac{d}{dy_0}\begin{pmatrix}\phi_1(y_0)\\ \psi_1(y_0)\end{pmatrix} = \frac{1}{y_0}\begin{pmatrix} -(y_0-1)^2-\lambda+1 & \frac{-y_0}{\lambda}(\lambda-y_0)(y_0+1) \\ 2\lambda(y_0-1) & (y_0-1)^2+\lambda-1\end{pmatrix} \times \begin{pmatrix}\phi_1(y_0)\\ \psi_1(y_0)\end{pmatrix} + B(y_0), \quad (57)$$

with

$$B(y_0) := \begin{pmatrix} \lambda^{-2}[-y_0 I_1 + (\lambda-y_0)I_2 + 2\lambda I_1 I_2] \\ -\lambda^{-1}\left[2(y_0-1)I_1 + \left(\frac{\lambda}{y_0} - 2(\lambda+1-y_0)\right)I_2 + \frac{2}{y_0}I_1 I_2\right]\end{pmatrix} \quad (58)$$

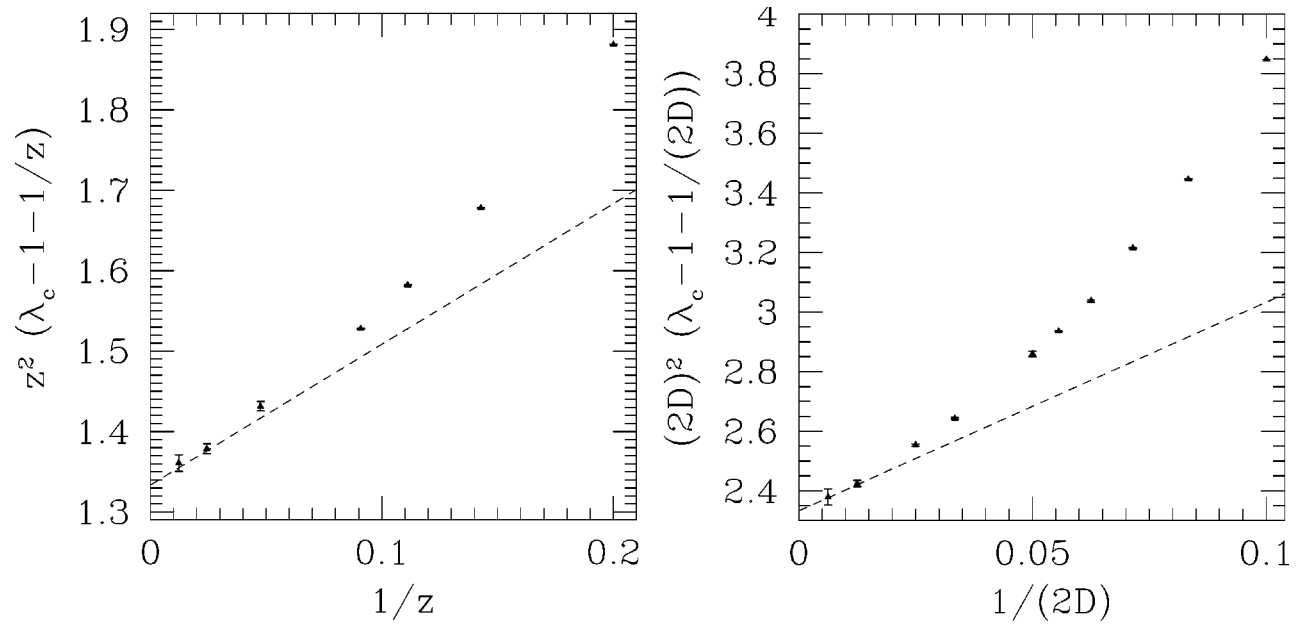

FIG. 4. Numerical data for the second-order correction in $1/z$ to $\lambda_C(z)$ for the Cayley tree (left panel) and the hypercubic lattice (right panel). The critical value λ_C is obtained from numerical experiments on the conserved contact process (CPP), see main text. Data are plotted as $z^2[\lambda_C(z)-1-1/z]$ vs $1/z$. The intercept a with the vertical axis ($z\to\infty$) compares very well with the theoretical predictions $a=4/3$ [Eq. (56), left] and 7/3 [Eq. (55), right]. Dashed lines are tentative linear fits (with fixed origin at $1/z=0$) of the data, whose slopes should be given by the $O(1/z^3)$ expansion. The estimate of λ for each z was obtained through an extrapolation of data for finite numbers of particles N (up to 4000) to infinite N. For each value of N, we ran 10 000 simulations and estimated error bars from the statistical fluctuations. The upper and lower values of $\lambda_C(z;N=\infty)$ were then obtained through a linear fit of $\lambda_C(z;1/N)$, and plotted at the extremities of the error bars.

and

$$I_1 := \left(\frac{\lambda-y_0}{y_0-1}\right)^{\alpha+2} \int_1^{y_0} dy_1 \frac{\lambda+1-y_1}{y_1-1}\left(\frac{y_1-1}{\lambda-y_1}\right)^{\alpha+2}, \quad (59)$$

$$I_2 := \left(\frac{y_0-1}{\lambda-y_0}\right)^{\alpha+2} \int_{y_0}^{\lambda} dy_1 \frac{y_1}{\lambda-y_1}\left(\frac{\lambda-y_1}{y_1-1}\right)^{\alpha+2}, \quad (60)$$

where α is defined by $\lambda=:1+2/\alpha$. The solutions of these equations diverge in $y_0=1$ for all initial conditions on ϕ_1,ψ_1 in $y_0=1$ except for $\phi_1(1)=-1/(2\lambda^2)$, $\psi_1(1)=0$ which precisely amounts to setting $\psi(y_0=1)=0$ and $\phi(y_0=1)=\rho^*$ up to order $1/z^2$. We choose these initial conditions in the following.

The resolution of the equations for ϕ_1 and ψ_1 can be done in part analytically and in part numerically. First, we treat the neighborhood of y_0 to characterize exactly the (nondivergent) singularity in this point. We have calculated the solutions up to the order $(y_0-1)^3\ln|y_0-1|$ included, which is sufficient to obtain the values of $\phi_1(1+\epsilon),\psi_1(1+\epsilon)$ slightly off (below or above) the singularity (with $\epsilon=\pm 0.001$ to 0.003) with a good numerical accuracy. Such an expansion amounts to a short-time expansion if one starts at $t=0$ from the typical state where the density of full sites is ρ^* and $y=1$. Then, we start to solve the differential equations from the value $y_0=1+\epsilon$ using a Runge-Kutta-Fehlberg procedure. Note that the coefficients of the EM for ϕ_1 and ψ_1 are rather simple, but the nonvanishing second member involves, for generic values of λ, hypergeometric functions. To simplify the numerical resolution and to make it more precise, we restricted ourselves to the case $\lambda=1+2/\alpha$ with α a positive integer, where these hypergeometric functions reduce to polynomials and logarithms.

This perturbative resolution yields a parametric representation of the large deviation distribution, $\pi^*(\rho)=\pi^*_{\rm MF}(\rho)+\pi_1^*(\rho)/z+O(1/z^2)$ with parameter y_0. More precisely, we have

$$\rho(y_0) := \phi(y_0) = \phi_0(y_0) + \frac{\phi_1(y_0)}{z} + O(1/z^2),$$

$$\pi(y_0) = \rho \ln y_0 - S_0(y_0) - \frac{\lambda^2}{z} S_1(y_0) + O(1/z^2), \quad (61)$$

where $S_0(y_0)=\ln y_0-(y_0-1)/\lambda$ and

$$S_1(y_0) = -\frac{1}{\lambda^4}\int_1^{y_0} dy_1 \frac{y_1}{\lambda-y_1}\left(\frac{\lambda-y_1}{y_1-1}\right)^{\alpha+2} \times \int_1^{y_1} dy_2 \frac{\lambda+1-y_2}{y_2-1}\left(\frac{y_2-1}{\lambda-y_2}\right)^{\alpha+2}. \quad (62)$$

The resulting curves for $\pi^*(\rho)$ are presented in Fig. 2. Apart from $\pi^*(\rho^*)=0$ given by Eqs. (53) and (54) and reached for $y_0=1$, another point of interest may be located analytically, namely $\pi^*(\rho=0)$, reached for $y_0=\lambda$. This is related to the lifetime of the metastable state, $t_{vac}\sim\exp[-N\pi^*(\rho=0)]$. Some values are listed in Table II for integer α.

To check the accuracy of our perturbative expansion for π^*, we have performed simulations of CP on six-

TABLE II. Some analytical values for the $1/z$ expansion of $\pi(\rho=0)$, the logarithm of the probability of reaching a configuration with vanishing density in the metastable state of the CP on a regular graph of coordination number z. Analytical calculation can be performed for values of $\lambda=1+2/\alpha$ with α a positive integer only, but $\pi(\rho=0)$ can be numerically estimated to order $1/z$ for other values of λ.

λ	$\pi(\rho=0)$	Decimal approximation
3	$-\ln 3+2/3+(-53/18+\pi^2/3)/z$	$-0.432+0.345/z$
2	$-\ln 2+1/2+(-107/36+\pi^2/3)/z$	$-0.193+0.318/z$
5/3	$-\ln(5/3)+2/5+(-5413/1800+\pi^2/3)/z$	$-0.111+0.283/z$
3/2	$-\ln(3/2)+1/3+(-1823/600+\pi^2/3)/z$	$-0.072+0.252/z$
7/5	$-\ln(7/5)+2/7+(-270281/88200+\pi^2/3)/z$	$-0.051+0.225/z$

dimensional hypercubic lattices with periodic boundary conditions. Sizes $N=L^6$ with L ranging from 3 to 6 are large enough that the system gets trapped for a time greater than the simulation run into the metastable state. We simulated the system starting from $\rho \ll \rho^*$ or $\rho \gg \rho^*$ until it reached equilibrium. The equilibration times (expressed as the number of elementary steps) was found to correspond to continuous times [53] t_{eq} ranging from 25 to 60. Then we run again the simulation for times $t=Mt_{eq}$ with very large values of M going from $M=2.5\times10^5$ for $L=6$ to $M=5\times10^7$ for $L=3$, and recorded the histogram of ρ over this time interval. This gives a very good approximation of the quasistationary distribution π^* since the system was already equilibrated. Numerical results for $\pi^*(\rho)$ are presented in Fig. 5. The maximum of $\pi^*(\rho)$ vanishes in the thermodynamic limit only, and the value ρ^* at which this maximum is reached is also subject to finite-size corrections. To make the comparison easier, we have vertically and horizontally shifted the experimental curves so that they all reach zero at the same value of ρ. Once this translation was done, the numerical and theoretical curves are in very good agreement, and are easily distinguishable from the mean-field curve (Fig. 5). This shows that the curvature (unaffected by the translations) of $\pi^*(\rho)$ and, hence, the amplitude of the fluctuations in the metastable state and its lifetime, is correctly predicted by our $1/z$ calculation.

V. CONCLUSION

In this paper, we have calculated the out-of-equilibrium distribution of densities of particles in the contact process on large regular lattices with degree z using a quantum field-theoretic formulation for the evolution operator. The calculation is based on a perturbative calculation of the effective potential for the density $\phi(t)$ and an instantonic field $\psi(t)$ as function of time t. Interestingly, this instantonic field naturally emerges from the parametrization of the quantum hard bosonic (or spins-$\frac{1}{2}$) states needed to represent the sets of occupation numbers.

The finite connectivity corrections to the mean-field case ($z=\infty$) lead to the appearance of memory kernels compensating the loss of information due to the tracking with time t of global fields $\phi(t),\psi(t)$ only. Though calculations may rapidly become involved, we have been able to show the very good agreement of the predictions they give with numerical experiments on the average density of particles and, more generally, the whole distribution of densities in the out-of-equilibrium metastable state of CP.

While the use of a quantum formalism was known to be very efficient to access universal quantities, e.g., the decay exponent of the density with time at criticality, the present study shows that nonuniversal quantities can be calculated too. We hope that this approach will turn out to be useful to the analysis of the numerous far-from-equilibrium systems encountered in physics or related fields. From this point of view, a remote but promising field of applications could be the analysis of algorithms in computer science where out-of-equilibrium dynamics over (discrete) variables abound, and metastability phenomena are present [54,55]. Hopefully our

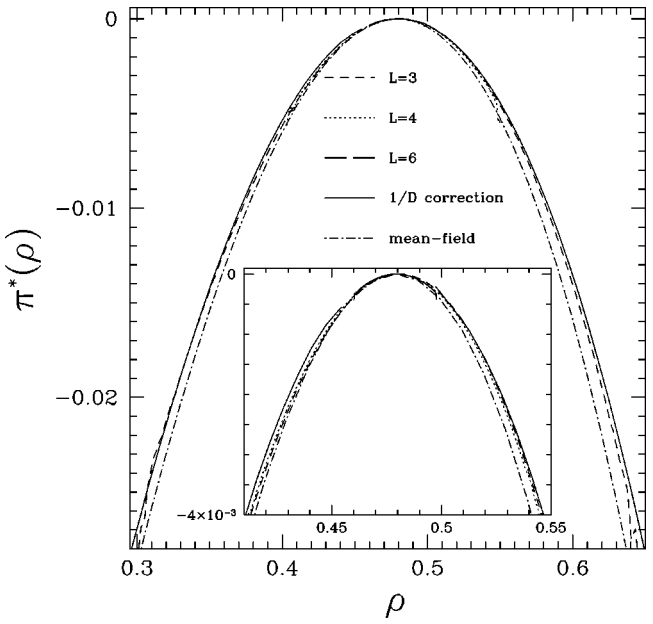

FIG. 5. Comparison, for $D=6$ and $\lambda=2$, between the $1/D$ predictions for the large deviation function $\pi^*(\rho)$ and numerical results for CP on hypercubic lattices with periodic boundary conditions of linear sizes $L=3$, 4, and 6. All curves were horizontally and vertically translated so that their maxima have the same coordinates $\rho^*,\pi^*=0$. Due to the relatively high dimensionality of these systems, the range of values of ρ explored during the simulations is very concentrated around ρ^* unless L is small. Note that the curves for different lattice sizes, once translated, seem to depend only weakly on L. Inset: enlargement of the top region; data compare well with the $1/D$ theoretical result (continuous line), and are clearly distinct from the mean-field result (dashed-dotted line).

approach will also permit to complete the average-case analysis of backtracking algorithms initiated in Refs. [56,57] through the systematic control of the non-Markovian effects ignored so far [58].

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APPENDIX: EMERGENCE OF MEMORY KERNEL WITH HIDDEN DEGREES OF FREEDOM

Consider two variables $x(t),y(t)$ obeying the Markovian evolution equations

$$\frac{dx}{dt}(t) = -x(t) + \beta y(t), \tag{A1}$$

$$\frac{dy}{dt}(t) = -\alpha y(t) + x(t), \tag{A2}$$

with initial conditions $x(0)=1$, $y(0)=0$. This system can be easily solved to give x and y as functions of time t. Assume instead we want to write an evolution equation for x only. Solving Eq. (A2), and plugging the resulting $y(t)$ in Eq. (A1), we obtain

$$\frac{dx}{dt}(t) = -x(t) + \beta \int_0^t \frac{d'}{dt} e^{-\alpha(t-t')} x(t'). \tag{A3}$$

As a result of the existence of a hidden degree of freedom y, the effective equation on x is not Markovian when $\beta \neq 0$, and includes a memory kernel whose time constant is that of the y variable.

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[32] A natural choice would have been $\langle a_i^\dagger a_i(t)\rangle = \overline{\phi}_i(t)$ and $\langle a_i(t)\rangle = \overline{\phi}_i(t)\exp[\overline{\psi}_i(t)]$. However this choice gives rise to a more complicated combinatorics in the $1/D$ expansion. $\hat{\chi}$, which appears aside $a^\dagger a$ on a different graph site in the expression of $\hat{W}$ is, in this respect, a better ''elementary'' operator. Furthermore, we will see that the expectation values of the other elementary operators evaluated with this choice will be consistent.
[33] This consistency statement holds also for other choices of Lagrange multipliers in $\hat{W}'$.
[34] The same expressions are also recovered if one optimizes directly $\Pi_{0,0}$ with respect to $h_i(t)$ and $g_i(t)$.
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[37] If $\phi(t)$ is always zero, $\psi(t)$ goes to 0 in a infinite time if $\psi(0) < \ln(\lambda)$, remains constant if $\psi(0)=0$ or $\psi(0)=\ln(\lambda)$, and goes to $+\infty$ in a finite time [all the shorter as $\psi(0)$ is large] if

$\psi(0) > \ln(\lambda)$. All these solutions have a vanishing action π_{MF}.

[38] The existence of the solution $\psi(t)=0$ to the EM is true beyond mean field, and is a consequence of the fact that the evolution operator $\hat{W}$ conserves the probability. The latter translates into $(\langle 0| + \langle 1|)\hat{W} = 0$ and, from Eq. (7), into $\tilde{W}(\vec{\phi}, \vec{\psi}=0)=0$ for any $\vec{\phi}$.

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