

2-2007

Quadratic Contact Process: Phase Separation with Interface-Orientation-Dependent Equistability

Da-Jiang Liu

Ames Laboratory, dajiang@fi.ameslab.gov

Xiaofang Guo

Iowa State University, mlmayor@iastate.edu

James W. Evans

Iowa State University, evans@ameslab.gov

Follow this and additional works at: http://lib.dr.iastate.edu/physastro_pubs



Part of the [Astrophysics and Astronomy Commons](#), [Mathematics Commons](#), and the [Physics Commons](#)

The complete bibliographic information for this item can be found at http://lib.dr.iastate.edu/physastro_pubs/205. For information on how to cite this item, please visit <http://lib.dr.iastate.edu/howtocite.html>.

This Article is brought to you for free and open access by the Physics and Astronomy at Iowa State University Digital Repository. It has been accepted for inclusion in Physics and Astronomy Publications by an authorized administrator of Iowa State University Digital Repository. For more information, please contact digirep@iastate.edu.

Quadratic Contact Process: Phase Separation with Interface-Orientation-Dependent Equistability

Abstract

The quadratic contact process is implemented on a square lattice as a model with random adsorption and correlated desorption requiring empty pairs of diagonal neighbors. The model exhibits a discontinuous phase transition between an active state and an absorbing state, but equistability between these states depends on the orientation of the separating interface. Correspondingly, for a generalized class of models, we find phase coexistence over a finite region of their two-dimensional parameter space. This is in stark contrast to behavior in equilibrium systems.

Keywords

computer simulation, ground state, mathematical models, molecular orientation, equistability, interface orientation, quadratic contact process, phase separation

Disciplines

Astrophysics and Astronomy | Mathematics | Physics

Comments

This article is from *Physical Review Letters* 98 (2007): 050601, doi: [10.1103/PhysRevLett.98.050601](https://doi.org/10.1103/PhysRevLett.98.050601). Posted with permission.

Quadratic Contact Process: Phase Separation with Interface-Orientation-Dependent Equistability

Da-Jiang Liu,¹ Xiaofang Guo,^{1,2} and J. W. Evans^{1,3}

¹Ames Laboratory, U. S. Department of Energy, Ames, Iowa 50011-3020, USA

²Department of Physics & Astronomy, Iowa State University, Ames, Iowa 50011, USA

³Department of Mathematics, Iowa State University, Ames, Iowa 50011, USA

(Received 10 October 2006; published 1 February 2007)

The quadratic contact process is implemented on a square lattice as a model with random adsorption and correlated desorption requiring empty pairs of diagonal neighbors. The model exhibits a discontinuous phase transition between an active state and an absorbing state, but equistability between these states depends on the orientation of the separating interface. Correspondingly, for a generalized class of models, we find phase coexistence over a finite region of their two-dimensional parameter space. This is in stark contrast to behavior in equilibrium systems.

DOI: [10.1103/PhysRevLett.98.050601](https://doi.org/10.1103/PhysRevLett.98.050601)

PACS numbers: 05.70.Fh, 02.50.Ey, 05.50.+q

Stochastic spatial models for cooperative processes have broad applicability in describing dynamics and pattern formation in systems involving, e.g., chemical reactions, population dynamics, spread of epidemics or information, and other ecological and sociological phenomena [1–5]. In contrast to traditional Hamiltonian systems [6], such non-equilibrium models often incorporate irreversible steps and thus are not constrained by detailed-balance conditions on the microscopic rates governing evolution. Consequently, these models can display a richer variety of spatiotemporal behavior. Nonetheless, their steady states often exhibit continuous and discontinuous phase transitions which appear analogous to equilibrium phase transitions in Hamiltonian systems [1–5]. However, the thermodynamic framework which facilitates the analysis of equilibrium transitions is lacking in the nonequilibrium case where understanding is limited.

Most investigation of nonequilibrium systems to date has focused on continuous transitions where the concept of universality carries over from equilibrium theory [1,4,5]. Less attention has been paid to discontinuous nonequilibrium transitions [3,4]. However, a well-known example of the latter provided is by the ZGB model [7] for the two-component monomer-dimer surface reaction where a transition to a monomer-poisoned absorbing state occurs for sufficiently high monomer adsorption rate. Various aspects of this transition have been characterized: epidemic properties [3,8], interface propagation and nucleation [9,10], and metastability [9,11]. Some unusual features likely reflect a small effective interface tension. Single-component models purportedly exhibiting discontinuous transitions have also been developed [2], although this behavior is sometimes disputed for lower dimensions [5].

Here, we consider single-component “contact models” which describe the spread of disease or information by nearest-neighbor (NN) interaction on a square lattice of sites [1,2]. Individuals are either sick or healthy. Sick individuals recover at a fixed rate, and healthy individuals

are infected by sick neighbors according to specific rules. We prefer to recast these models in the language of adsorption-desorption where sick (healthy) corresponds to an empty (filled) site. This facilitates comparison with classic equilibrium adsorption-desorption models for interacting adlayers. In the standard contact process (SCP), particles adsorb randomly on the empty sites of a lattice at rate or “pressure”, p , and desorb at a rate proportional to the number of empty NN sites. In the quadratic contact process (QCP), again particles adsorb randomly on empty sites at rate, p , but now desorb at a rate $k/4$, where k equals the number of diagonally adjacent empty pairs of NN sites [2]. Thus, $k = 0, 0, 2$, and 4 for $0, 1, 3$, and 4 empty NN sites, respectively, and $k = 1$ (0) for 2 empty NN sites which are diagonally adjacent (on opposite sides of the particle).

The SCP and QCP are in turn often identified with Schlögl’s 1st and 2nd models for autocatalytic kinetics, respectively [2,12]: $X \leftrightarrow 2X$ and $X \rightarrow \emptyset$ for the 1st model, and $2X \leftrightarrow 3X$ and $X \rightarrow \emptyset$ for the 2nd model, where $X \rightarrow \emptyset$ denotes annihilation of a particle X . The mean-field kinetics is quadratic (cubic) for the 1st (2nd) model suggesting a continuous (discontinuous) transition to the vacuum state. Indeed, Schlögl’s 1st model does exhibit a continuous transition to the vacuum state, and correspondingly the SCP exhibits a continuous poisoning transition to a completely covered surface in the directed percolation universality class [1]. One careful study of a cellular-automata realization of Schlögl’s 2nd model [13] reported a continuous transition (for spatial dimension $D = 1-3$). However, model behavior will depend on the specific discrete realization.

In this Letter, we show that the QCP on a square lattice does in fact exhibit a discontinuous transition, i.e., phase separation, between an active state with low coverage and an absorbing state corresponding to a completely covered surface. However, in marked contrast to equilibrium systems, the adsorption rate or pressure for equistability be-

tween these states, p_{eq} , depends on the orientation of the interface separating them. This implies that bistability exists over a finite range of pressure. Furthermore, for a generalized class of models, we find a corresponding phase coexistence over a finite region of their two-dimensional parameter space.

Our model analysis is performed using kinetic Monte Carlo (KMC) simulation on $L_x \times L_y$ site square-lattice systems with periodic boundary conditions. In conventional constant- p KMC simulation of the QCP, one specifies an adsorption rate, p , and then runs the simulation implementing adsorption and desorption with the appropriate rates to determine dynamics and steady-state behavior. For lower p , the system reaches a stable low-coverage active state with a steady-state coverage satisfying $\theta(p) \approx p + O(p^2)$. For higher p above about 0.1, the system quickly reaches a stable absorbing or poisoned state with $\theta(p) \equiv 1$. See below.

In constant-coverage (CC) simulation [14], one specifies a target coverage θ and runs the simulation attempting to adsorb (desorb) if the actual coverage is below (above) the target θ . The fraction of adsorption attempts yields the pressure $p = p(\theta)$. CC and constant- p simulation become equivalent for sufficiently large systems. The CC approach is particularly useful for discontinuous transitions where specifying θ anywhere in the range of the discontinuous jump in θ versus p yields the same equistability pressure, p_{eq} . Here, we further exploit the CC approach to search for dependence of $p_{\text{eq}} = p_{\text{eq}}(S)$ on the slope, S , of the interface between active and absorbing phases. To this end, we perform simulations in rectangular systems with $L_y = SL_x$ starting from an initial filled strip of the absorbing state of slope S for target $\theta = 0.5$. During simulation, the strip equilibrates but remains stable, its mean slope S being preserved due to the boundary conditions. Simulations performed with different L_y to check for finite-size effects indicate a clear slope dependence: $p_{\text{eq}}(L_y \rightarrow \infty) = 0.09443, 0.09400, \text{ and } 0.09283 (\pm 0.00003)$, for $S = 1, 2, \text{ and } 4$, respectively. See Fig. 1(a). The special case $S = \infty$ is discussed below.

An independent assessment of equistability, as well as a more comprehensive analysis of interface propagation, can be obtained from standard constant- p simulations. Starting from an initial filled strip with slope S , where $1 \leq S < \infty$ in a rectangular system with $L_y = SL_x$, one monitors the rate of growth or shrinkage of the strip to obtain the propagation velocity, $V(S, p)$. Results for $V(S, p)$ versus p are shown in Fig. 2. For $0 \leq p < p_{\text{eq}}(S)$, the more stable active state displaces the less stable absorbing state and $V(S, p) > 0$. The opposite applies for $p > p_{\text{eq}}(S)$ where $V(S, p) < 0$. Estimates of $p_{\text{eq}}(S)$ from this plot are entirely consistent with but less precise than those above from CC simulation. For each S , $V(S, p)$ increases smoothly with decreasing p to a maximum at $p = 0$. As an aside, we note that interface propagation for general S in the QCP when $p = 0$ (i.e., irreversible shrinkage of an absorbing

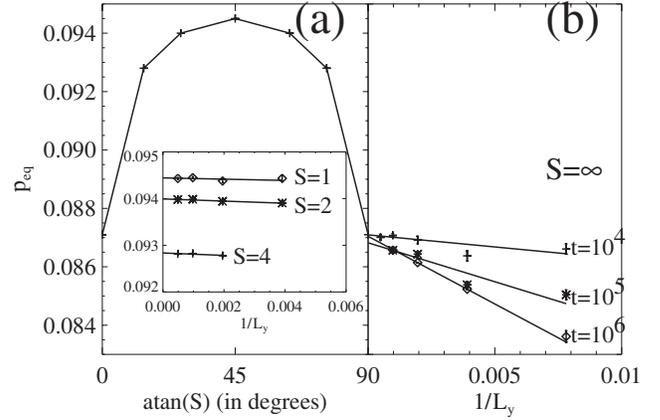


FIG. 1. (a) Dependence of p_{eq} on interface slope S . Inset shows CC simulation analysis of system size effects for $S = 1, 2, \text{ and } 4$. (b) Analysis of system size and CC simulation time (shown in MCS) on estimates for $p_{\text{eq}}(S = \infty)$.

strip) maps onto the exactly solvable 1 + 1D single-step deposition model for irreversible growth on a sloped surfaces [15]. Previous results for the latter imply that $V(S = 1, p = 0) = 1/(8\sqrt{2})$ and $V(S, p = 0) \propto S(S + 1)^{-1}(S^2 + 1)^{-1/2}$ for $S > 1$.

Next, we consider the “delicate” case of evolution of a vertical strip of filled sites, i.e., an interface with slope $S = \infty$. As a direct consequence of the QCP desorption rules, particles within completely filled vertical columns of this strip can never desorb. Thus, the strip can never erode for any $p \geq 0$. However, let us assume that such a strip in an infinite system is stable against expansion for $0 \leq p \leq p_{\text{eq}}(S = \infty)$. Then, we note that simulated behavior in this p regime is “corrupted” in finite-size systems. Why? Consider the partially completed columns adjacent to the completed columns of the strip. Completion of each such column corresponds to falling into a 1D absorbing state. Consequently, this event must eventually occur with probability unity in a finite system. For conventional simulations, this results in strip expansion for any $p > 0$. In CC simu-

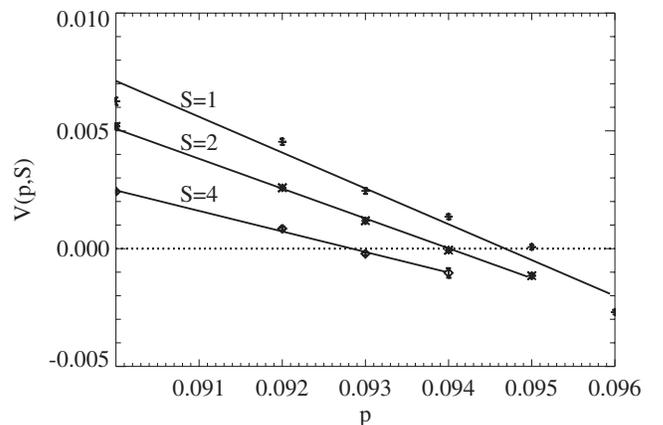


FIG. 2. Interface propagation velocity, $V(p, S)$, versus p from constant- p simulations for $S = 1, 2, \text{ and } 4$.

lations, this results in a decrease in the coverage of the active state and a corresponding slow decrease in the effective pressure with increasing time. To systematically remove such finite-size effects, we perform CC simulations for a sequence of systems with $L_y = 2^n L_x$ containing a vertical interface of length $2^n L_x$, and extrapolate behavior $n \rightarrow \infty$. We also compare behavior for different simulation times (longer times yield lower p). Results shown in Fig. 1(b) indicate that $p_{\text{eq}}(S = \infty) \approx 0.0869(\pm 0.0004)$, for $L_y \rightarrow \infty$.

For additional insight into vertical interface evolution, we consider the dynamics of the first incomplete column adjacent to a complete edge column bordering the absorbing state. There are three types of occupied sites in this column: (i) particles in the interior of vertical strings of two or more filled sites which cannot desorb; (ii) particles at the ends of vertical strings which have one empty neighbor in the same column, and which desorb at rate $Q_e/4$; (iii) particles for which the neighboring upper and lower sites are both empty, and which desorb at rate $Q_e/2$. Here, Q_e denotes the conditional probability that the NN site in the neighboring incomplete column is empty, where we neglect any dependence of this conditional probability on other details of the local environment. Then, the process of column completion maps onto a classic 1D contact process. Based on previous simulation studies of this 1D contact process [1], it follows that column completion displays a continuous transition to an absorbing state for $p = p_{\text{eq}}(1D) = 0.1516Q_e$ which we identify as $p_{\text{eq}}(S = \infty)$.

It remains to determine Q_e at the relevant equestability point where $\theta = \theta_{\text{eq}} \approx 0.17$ taken from Fig. 3. The simplest site-approximation sets $Q_e = 1 - \theta_{\text{eq}} \approx 0.83$, so $p_{\text{eq}}(1D) \approx 0.126$ (site). A pair-approximation for the QCP (described elsewhere) yields $Q_e = (1 - \theta_{\text{eq}})/(1 + \theta_{\text{eq}}) \approx 0.71$, so $p_{\text{eq}}(1D) \approx 0.108$ (pair). Alternatively, one can utilize simulations to directly assess Q_e . We have done this using CC simulations starting with a narrow vertical column of length 1024 in a 256×1024 site system. We set a target $\theta = 0.25$, and collect statistics on Q_e once the number of completed rows in the growing absorbing strip reaches around 20, so the local coverage in the active state is just above 0.17. From this analysis, we obtain $Q_e \approx 0.58$, so that $p_{\text{eq}}(1D) \approx 0.088$ (simulation) consistent with the above estimate.

From the above analyses, we conclude that $p_{\text{eq}}(S)$ decreases monotonically with increasing S from a maximum of $p_{\text{eq}}(S = 1) \approx 0.0944$ to a minimum of $p_{\text{eq}}(S = \infty) \approx 0.087$. This is in marked contrast to behavior in equilibrium adsorption-desorption systems including appropriate attractive interactions. Here, a single equestability pressure exists corresponding to equality of the chemical potential for the coexisting 2D dilute and dense phases. A comprehensive illustration of steady-state behavior in the QCP is provided by Fig. 3(a): a unique stable absorbing state exists for $p > p_{\text{eq}}(S = 1)$; a stable active state exists for $p < p_{\text{eq}}(S = \infty)$; both the absorbing and active states are stable

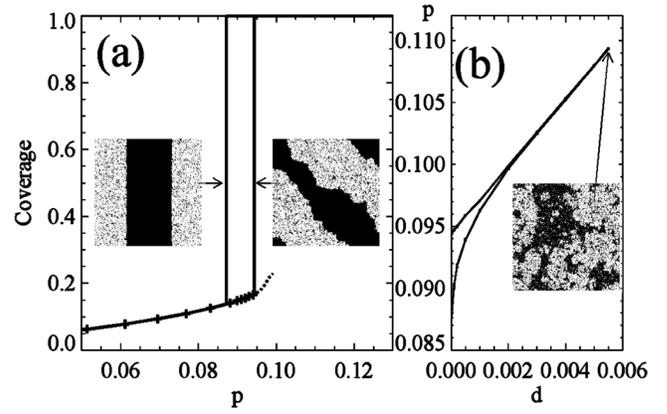


FIG. 3. (a) Steady-state coverage behavior for the QCP. The dotted line gives one metastable extension of the active state. Vertical lines indicate the boundaries of true bistability, and insets indicate associated equestable interface configurations. (b) Bistability region for the generalized QCP with an additional pathway for random desorption at rate d . The inset shows a configuration near the Ising-like critical point.

for $p_{\text{eq}}(S = \infty) < p < p_{\text{eq}}(S = 1)$ in that either can displace the other depending on interface orientation, i.e., there is true bistability. For $p < p_{\text{eq}}(S = \infty)$ the absorbing state is stable against isolated active droplets (see below). As for equilibrium systems [16], presumably the active state cannot be analytically extended to a unique metastable state, but there will exist a smooth C^∞ family of extensions for $p > p_{\text{eq}}(S = 1)$. One of these [17] is indicated in Fig. 3. No precisely defined spinodal point terminates this metastable state, but the poisoning kinetics above the metastable region are found to depend strongly on the distance to an effective spinodal [9], $p_s \approx 0.100(\pm 0.002)$.

Further insight into the origin of true bistability over a finite range of p comes from an analysis of the dynamics of droplets of one phase embedded in the other. First, consider the evolution of droplets of the absorbing state embedded in the active state when $p_{\text{eq}}(S = \infty) < p < p_{\text{eq}}(S = 1)$. Since we claim that active state is stable in this regime, we must rationalize why such (spontaneously forming) droplets ultimately disappear even though the absorbing state is stable. To focus on a “worst case scenario”, consider a square-shaped droplet having sides orientated with slopes $S = 0$ and $S = \infty$. Then, since $p > p_{\text{eq}}(S = \infty)$, the sides of this droplet will initially tend to expand. If growth at the corners is inhibited, then a roughly octagonal shaped droplet will develop. Subsequently, the facets with slope $S \approx \pm 1$ will tend to contract, since $p < p_{\text{eq}}(S = 1)$, and the sides with $S = 0$ or ∞ will grow out yielding a diamond shape droplet which will naturally shrink. (Large fluctuations hide this progression in geometric shapes. Even with an initial 64×64 site droplet and “high” $p = 0.094$, shrinkage starting at the corners is more evident than growth of the $S = 0$ and $S = \infty$ sides.) Of course, the active state is unstable and droplets grow with finite probability for $p > p_{\text{eq}}(S = 1)$.

Second, consider droplets of the active phase (or empty droplets) embedded in absorbing phase. A special feature of the desorption rules in the QCP is that such a droplet can never grow outside of a rectangle containing the droplet. Thus, trivially, the absorbing state is stable against such isolated droplets which must disappear for any $p > 0$, a feature already noted by Durrett [2]. However, perturbations of the model dynamics to remove the above special feature allow growth of an empty droplet with finite probability for $p < p_{\text{eq}}(S = \infty)$ below the true bistable window (see below).

How general is the feature of a finite range of true bistability in nonequilibrium lattice-gas adsorption-desorption type models? It is natural to generalize the QCP model to include an additional pathway for random desorption characterized by “small” rate $d > 0$. In this model, the high- θ stable state is no longer absorbing. The system states are parameterized by both pressure, p , and the temperaturelike variable d ($d = 0$ recovering the QCP), so one can make a more complete comparison with equilibrium adsorption-desorption models. We find that the finite region of bistability persists for $d > 0$, but shrinks to zero at a critical cusp point, $d = d_c$. See Fig. 3(b). The boundaries of this finite region of bistability were obtained from CC simulations for interfaces with slope $S = 1$ and $S = \infty$, respectively. Detailed finite-size-scaling analysis of fluctuation behavior near the nonequilibrium critical point [11,18] indicates Ising-like behavior with $d_c = 0.055$ and $p = p_c = 0.1090$. As an aside, we mention another generalized model motivated by the standard contact process: here additional desorption occurs with rate $dm/4$ for particles with m NN empty sites (in addition to the QCP pathway). This model preserves the completely covered surface as an absorbing steady-state, and also has a finite region of bistability extending for $d > 0$ similar to the first generalized model.

More broadly, the phenomenon of true bistability or generic two-phase coexistence has been noted in other nonequilibrium models. However, typically, it derives from a rather severe departure from traditional Hamiltonian-based dynamics. One example is Toom’s North-East-Center synchronous stochastic cellular automata model which introduces an explicit artificial asymmetry into dynamic “voting” rules [19]. Continuum analogues incorporating this asymmetry also exhibit true bistability [20]. Here, behavior can be rationalized in terms of very unusual droplet dynamics. Another example is provided by models for interface pinning-depinning transitions where true bistability can derive from the feature that a greater driving force is required to depin an interface than to maintain motion [21]. Finally, we note that metastability is enhanced in nonequilibrium adsorption-desorption type models by introducing particle hopping [9,22]. However, true bistability is only achieved in the rapid-hopping hydrodynamic limit [22].

In conclusion, we have shown that the QCP on a square lattice exhibits a discontinuous phase transition with true bistability. This QCP is closer to traditional equilibrium models than Toom-type models. The origin of its bistability is more delicate, deriving from a quite weak dependence of equistability on interface orientation.

This work was supported by the U.S. DOE-BES Chemical Sciences Division and performed at Ames Laboratory operated by ISU under Contract No. W-7405-Eng-82.

-
- [1] J. Marro and R. Dickman, *Nonequilibrium Phase Transitions in Lattice Models* (Cambridge University Press, Cambridge, England, 1999).
 - [2] R. Durrett, *SIAM Rev.* **41**, 677 (1999).
 - [3] E. Loscar and E. V. Albano, *Rep. Prog. Phys.* **66**, 1343 (2003).
 - [4] G. Ódor, *Rev. Mod. Phys.* **76**, 663 (2004).
 - [5] H. Hinrichsen, *Adv. Phys.* **49**, 815 (2000).
 - [6] J.D. Gunton, M.S. Miguel, and P.S. Sahni, *Phase Transitions and Critical Phenomena* (Academic, New York, 1983), Vol. 8.
 - [7] R. M. Ziff, E. Gulari, and Y. Barshad, *Phys. Rev. Lett.* **56**, 2553 (1986).
 - [8] J. W. Evans and M. S. Miesch, *Phys. Rev. Lett.* **66**, 833 (1991).
 - [9] J. W. Evans and T. R. Ray, *Phys. Rev. E* **50**, 4302 (1994).
 - [10] R. H. Goodman, D. S. Graff, L. M. Sander, P. Leroux-Hugon, and E. Clément, *Phys. Rev. E* **52**, 5904 (1995).
 - [11] E. Machado, G. M. Buendia, and P. A. Rikvold, *Phys. Rev. E* **71**, 031603 (2005).
 - [12] F. Schlögl, *Z. Phys.* **253**, 147 (1972).
 - [13] P. Grassberger, *Z. Phys. B* **47**, 365 (1982).
 - [14] R. M. Ziff and B. J. Brosilow, *Phys. Rev. A* **46**, 4630 (1992).
 - [15] J. Krug and H. Spohn, *Europhys. Lett.* **8**, 219 (1989).
 - [16] R. H. Schonmann and S. B. Shlosman, *Commun. Math. Phys.* **194**, 389 (1998).
 - [17] For $\delta p = p - p_{\text{eq}}(S = 1) > 0$, critical droplets of the absorbing state are created at rate $k \propto \exp(-\lambda_c/\delta p)$ with $\lambda_c \approx 0.02$, and then grow with velocity $v \propto \delta p$. Avrami theory implies a characteristic time for nucleation-mediated poisoning satisfying $\tau_{\text{nuc}} \sim v^{-2/3} k^{-1/3} \sim \exp[\lambda_c/(3\delta p)]$. Then, C^∞ extensions can be generated by constant- p evolution from an empty surface for a time $\tau_{\text{sim}} \sim \exp[\lambda/(3\delta p)]$ with $\lambda < \lambda_c$.
 - [18] D.-J. Liu, N. Pavlenko, and J. W. Evans, *J. Stat. Phys.* **114**, 101 (2004).
 - [19] A. L. Toom, in *Multicomponent Random Systems*, edited by R. L. Dobrushin and Y. G. Sinai, *Advances in Probability and Related Topics*, Vol. 6 (Marcel Dekker, New York, 1980), Chap. 18, p. 549.
 - [20] Y. He, C. Jayaprakash, and G. Grinstein, *Phys. Rev. A* **42**, 3348 (1990).
 - [21] M. A. Muñoz, F. de los Santos, and M. M. T. da Gama, *Eur. Phys. J. B* **43**, 73 (2005).
 - [22] J. W. Evans, D.-J. Liu, and M. Tammaro, *Chaos* **12**, 131 (2002).