Characterization of the phase transitions in the Ziff-Gulari-Barshad model with spatial diffusion under two different prescriptions

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In this work, we modify the Ziff-Gurari-Barshad (ZGB) model by including the spatial diffusion of oxygen atoms and of carbon monoxide molecules, both adsorbed on the lattice, in order to study its effect on the continuous and discontinuous phase transitions of the model through time dependent Monte Carlo simulations. We use an optimization method based on a concept known as coefficient of determination to construct color maps and obtain the phase transitions when the parameters of the model vary, i.e., the rates of adsorption of carbon monoxide and of diffusion. This method was proposed recently to locate the non-equilibrium second-order phase transitions and has been successfully used in both systems: with defined Hamiltonian and with absorbing states. We also use two different approaches: in the first one, we consider or the adsorption process OR (Exclusive OR) the diffusion process in each trial (never both in the same trial); in the second one, we consider the adsorption process OR the diffusion process in each trial (same trial can include both). Both approaches present two interesting results: the continuous phase transition point of the original ZGB model disappears when the diffusion rate increases. However, the discontinuous phase transition is not destroyed even when the diffusion rate approaches to 1, indicating that there exists a line of discontinuous phase transition points.

Keywords: Spatial diffusion, ZGB model; Refinement process; Models with absorbent steady state; Time-dependent Monte Carlo simulations

I. INTRODUCTION

In a pioneering work back in 1986, Ziff, Gulari, and Barshad proposed a model that mimics reactions on a catalytic surface [1] to describe some nonequilibrium aspects of the production of carbon dioxide \((\text{CO}_2)\) molecules through the reaction of carbon monoxide \((\text{CO})\) molecules with oxygen \((\text{O})\) atoms. This stochastic model, also known as ZGB model, has attracted much interest due to its simplicity and rich phase diagram with continuous and discontinuous phase transitions which separate absorbing phases from a reactive steady state phase [2,3].

In addition to the scientific interest, the reason for the increasingly study of catalytic reaction models on surfaces lies in the possible applications to the technology [5,7]. In this respect, the ZGB model has been vastly studied nowadays and is considered a prototype for the study on catalytic surfaces due to its inherent reaction processes that also take place in industry which deals with oxidation of CO on transition-metal catalysts.

Nevertheless, some aspects of the catalytic reaction can not be explained by this model. While some experimental works on platinum confirm the existence of discontinuous irreversible phase transitions (IPT) in the catalytic oxidation of CO [8,12], there is no experimental evidence of the continuous IPT. From the theoretical point of view, the continuous phase transition has been studied by several authors and the results support that this transition belongs to the directed percolation (DP) universality class [13,14].

Modified versions of the ZGB model has been proposed in order to obtain systems with actual catalytic processes and/or to eliminate the continuous phase transition of the original model. Some modifications include CO desorption [11,15,20], diffusion [4,11,18,19,21], impurities [22,23], attractive and repulsive interactions between the adsorbed molecules [27], surfaces of different geometries [1,23] and with hard oxygen boundary conditions [29], etc. In addition, it has been studied through several techniques, such as simulations, mean-field theories, series analysis, etc [7].

In this paper, we perform short-time Monte Carlo (MC) simulations in order to explore the behavior of the phase transitions of the ZGB model when both O atoms and CO molecules adsorbed on the catalytic surface are able to move, i.e., when diffusion is allowed. By using time-dependent MC simulations and an optimization method known as coefficient of determination [20], we construct maps and obtain the transitions when the parameters of the model varies. As shown in the next section, the only two parameters considered in our study are the rates of adsorption of CO molecules and the rates of diffusion. This technique has been used in the study of reversible systems [21,34] and was considered recently in the study of an epidemic model to determine its critical immunization probability [35], and to obtain the continuous transition point and the upper spinodal point of the ZGB model [36]. In addition, two different ways of performing the trials are proposed.

Our work is organized as follows: In the next section, we present the model with diffusion and show the two manners of moving the atoms/molecules considered in this paper. In Sec. [11] we describe some finite-size scaling relations in nonequilibrium systems with absorbing states.
II. THE MODEL

In this work, we study the dynamical behavior of a modified version of the ZGB model, first devised in 1986 by R.M. Ziff, E. Gulari, and Y. Barshad [1], in order to describe the production of carbon dioxide (CO$_2$) molecules through the reaction of carbon monoxide (CO) molecules and oxygen (O) atoms on a catalytic surface. In other words, the ZGB model is a dimer-monomer model which simulates the catalysis between the carbon monoxide molecule and the oxygen atom [1, 37]. In our approach, in addition to the well-known reactions presented in the original model,

\[
\begin{align*}
&\text{CO}(g) + V \rightarrow \text{CO}(a), \\
&\text{O}_2(g) + 2V \rightarrow 2\text{O}(a), \\
&\text{CO}(a) + \text{O}(a) \rightarrow \text{CO}_2(g) + 2V,
\end{align*}
\]

there are other two reactions that are related to the diffusion of CO molecules or O atoms adsorbed on the surface:

\[
\begin{align*}
&\text{O}_2(a) + V_j \rightarrow \text{O}(a) + V_i, \\
&\text{CO}_2(a) + V_j \rightarrow \text{CO}(a) + V_i.
\end{align*}
\]

In these reactions, V stands for vacant sites on the surface, and g and a refer, respectively, to the gas and adsorbed phases of the atoms/molecules. The indexes i and j stand for nearest neighbor sites and are explicitly presented in Eqs. (1) and (3) in order to represent the diffusion of the atoms/molecules if there exists some vacant site in the vicinity of them. As shown in the above equations, O$_2$ and CO$_2$ molecules exist only in the gas phase (g) while O atoms are present only in the adsorbed phase (a) and CO molecules are able to be in both phases.

In order to simulate such a model, one can think of the catalytic surface as a regular square lattice with its sites occupied by CO molecules or by O atoms or even be empty (V). The simulation is carried out as follows [1, 7, 38]: By following Eq. (1), the CO molecule in the gas phase is chosen to impinge on the surface with a rate $y_{\text{CO}}$. The molecule strikes the lattice in a site previously chosen at random. If the site is vacant (V), then the CO molecule is adsorbed on it. Otherwise, if the site is occupied by a CO molecule or by an O atom, the trial ends, the CO molecule returns to the gas phase, and a new molecule is chosen. On the other hand, from Eq. (2), if an O$_2$ molecule in the gas phase is chosen to hit the lattice, it does so at a rate $y_{\text{O}_2} = 1 - y_{\text{CO}}$. In this case, a nearest-neighbor pair of sites is chosen at random, and, if both sites are vacant (2V), the O$_2$ molecule dissociates into a pair of O atoms and are adsorbed on the chosen lattice sites. However, if one or both sites are occupied, the trial ends, the O$_2$ molecule returns to the gas phase, and a new molecule is chosen. As can be seen, these rates are relative ones, $y_{\text{CO}} + y_{\text{O}_2} = 1$, and the model, as presented in Ref. [1], has a single free parameter: $y = y_{\text{CO}}$. Eq. (3) is related to the reaction between the O atom and the CO molecule, both adsorbed on the lattice. Immediately after each adsorption event [Eqs. (1) and (3)], the nearest-neighbor sites of the adsorbed molecule/atom are checked. If an O–CO pair is found, a CO$_2$ molecule is formed and quits the lattice, leaving two empty sites on it. However, if there is the possibility of formation of two or more O–CO pairs, a pair is chosen at random to quit the lattice. The last two equations represent the diffusion process proposed in this work: A site i is chosen at random and, if it is occupied by an O atom or by a CO molecule, Eqs. (4) and (5) respectively, a nearest-neighbor site j is also chosen at random. If j is vacant, the atom/molecule moves to it with a rate $p$ leaving the site i empty. It is worth to mention that if there is diffusion, Eq. (3) must be used again to verify if there is formation of CO$_2$ molecule or not.

The ZGB model possesses two phase transitions. The first one is a continuous phase transition and occurs at the critical point $y_c \approx 0.3874$ [30, 39]. The second transition is discontinuous and occurs at $y_c \approx 0.5256$ [40]. For $0 \leq y < y_1$, the surface becomes irreversibly poisoned (saturated) by O atoms (O–poisoned state) and for $y_2 < y < 1$ the surface becomes irreversibly poisoned by CO molecules (CO–poisoned state). The poisoned state, or absorbing phase, represents states in which, once reached, the systems become trapped and cannot escape anymore. On the other hand, for $y_1 < y < y_2$ there exists a reactive steady state with sustainable production of CO$_2$ molecules. So, both $y_1$ and $y_2$ are irreversible phase transition (IPT) points between the reactive and poisoned states.

In this study, we are wondering if the diffusion of the atoms/molecules influences the first and second order phase transitions of the ZGB model. In order to answer this question, we separate the MC simulations into two different moments: the first moment is related to the diffusion process given by Eqs. (1) and (5), and the second one deals with the catalytic reaction given by Eqs. (1), (2), and (3). In addition, we proposed two different ways of performing the simulations:

1. **Algorithm I: Diffusion process “XOR” adsorption process** – With a rate $p$, the diffusion process is chosen (first moment). On the other hand, the adsorption process occurs with a rate $1 - p$, and, in this case, the process is governed by the parameter $y$ as well as by the rules defined previously (second moment). In summary, both the diffusion and adsorption processes are allowed but not in the same trial.

2. **Algorithm II: Diffusion process “OR” adsorption process** – The diffusion process of the atoms/molecules occurs with a rate $p$ and then the
adsorption process can occur with a rate $y$. In summary, both processes can occur in the same trial.

III. TIME DEPENDENT MONTE CARLO SIMULATIONS

In this work, we carry out short-time MC simulations to study the behavior of the ZGB model with diffusion of the atoms/molecules adsorbed on the lattice. In order to perform the numerical simulations, we take into consideration that, for systems belonging to the DP universality class, the finite-size scaling near criticality can be described by:

$$\langle \rho(t) \rangle \sim t^{-\beta/\nu_\parallel} f((y - y_c) t^{1/\nu_\parallel}, t^{d/\nu} L^{-d}, \rho_0 t^{\beta/\nu_\parallel + \theta}),$$

where $\rho$ is the density of $CO$ molecules, $\cdots$ stands for the average on different evolutions of the system, $d$ is the dimension of the system (for the ZGB model, $d = 2$), $L$ is its linear size of a regular square lattice, and $t$ is the time. The indexes $z = \nu_\parallel/\nu_\perp$ and $\theta = \frac{d}{2} - \frac{2\beta}{\nu_\parallel}$ are dynamic critical exponents, and $\beta$, $\nu_\parallel$, and $\nu_\perp$ are static ones. Here, $y - y_c$ denotes the distance of a point $y$ to the critical point, $y_c$, which governs the algebraic behaviors of the two independent correlation lengths: the spatial one which behaves as $\xi_\perp \sim (y - y_c)^{-\nu_\perp}$ and the temporal one, $\xi_\parallel \sim (y - y_c)^{-\nu_\parallel}$.

The density of $CO$ molecules adsorbed on the lattice is given by

$$\rho(t) = \frac{1}{L^d} \sum_{j=1}^{L^d} s_j,$$

and $s_j = 1$ when the sites $j$ are occupied by $CO$ molecules, otherwise, it is equal to zero.

As shown in Ref. [38], the dynamic and static critical exponents of the model can be obtained by using the Eq. [9] and performing time-dependent MC simulations with two different initial conditions $\rho(0) = \rho_0$: (i) the lattice is completely empty, i.e. there exist only vacant sites ($\rho_0 = 0$) and (ii) the lattice is completely filled with $O$ atoms but a random site which remains empty ($\rho_0 = 1/L^2$). When considering the first condition, one obtains

$$\langle \rho \rangle (t) \sim t^\lambda,$$

where $\lambda = -\beta/\nu_\parallel$, and the second condition produces

$$\langle \rho \rangle (t) \sim \rho_0 t^\theta = \rho_0 t^{\left(\frac{d}{2} - \frac{\beta}{\nu_\parallel}\right)}.$$

The numerical computing of the exponents $\lambda$, $\beta$, and $\nu_\parallel$, follows a straightforward procedure: First, by considering these two different initial conditions, it is possible to obtain the exponent $z$ in a very simple way, leading to the following power law $F_2(t) = \langle \rho \rangle_{\rho_0 = 1/L} (t) / \langle \rho \rangle_{\rho_0 = 1} (t) \sim t^{d/z}$. In addition to the analysis of these power laws in the study of the original ZGB model [38], this idea has been applied successfully in a large number of spin systems: for example, the Ising model, the $q = 3$ and $q = 4$ Potts models [41], Heisenberg model [42] and even for models based on the generalized Tsallis statistics [43]. It was also introduced recently in systems without defined Hamiltonian, as can be seen in Ref. [44]. Second, in order to compute $\nu_\parallel$, another power law is obtained when taking into account the following derivative [45]:

$$D(t) = \frac{\partial \ln \langle \rho \rangle}{\partial \sqrt{t}}_{\rho = \rho_c}$$

which is numerically represented by

$$D(t) = \frac{1}{2\delta} \ln \left( \frac{\langle \rho \rangle(y + \delta)}{\langle \rho \rangle(y - \delta)} \right),$$

where $\delta$ is a tiny perturbation needed to move the system slightly off the criticality, yielding a power law decay that only depends on $\nu_\parallel$, i.e.,

$$D(t) = t^{\nu_\parallel}.$$

However to determine these exponents by using this tool of power laws, the critical parameters must be accurately determined. Can this task also be determined via time-dependent MC simulations? In this paper we are concerned with the influence of the diffusion on the existence of the continuous and discontinuous irreversible phase transitions of the ZGB model. So, instead of focusing on the estimate of the critical exponents, we decided to take into account a very simple and efficient optimization method to obtain an overview of the phase transitions when the rate of adsorption of $CO$ molecules ($y$) on the lattice and the rate of diffusion $p$ vary from zero to one, i.e., $0 \leq y \leq 1$ and $0 \leq p \leq 1$.

This method considers the robustness of the power laws, and it is based on a quantity known as coefficient of determination. It is given by

$$r = \frac{\sum_{t=1}^{N_{MC}} (\ln \langle \rho \rangle - a - b \ln t)^2}{\sum_{t=1}^{N_{MC}} (\ln \langle \rho \rangle - \ln \langle \rho \rangle (t))^2},$$

where $\rho = \rho(t)$ is obtained for each pair $(y, p)$, $N_{MC}$ is the number of MC steps, $a$ and $b$ are, respectively, the intercept and the slope of a linear function, and $\ln \langle \rho \rangle = (1/N_{MC}) \sum_{t=1}^{N_{MC}} \ln \langle \rho \rangle (t)$. Here differently from $\Omega = (1/N_{MC}) \sum_{t=1}^{N_{MC}} O(t)$ which denotes an average over the MC steps, $\langle O \rangle (t) = (1/N_{run}) \sum_{i=1}^{N_{run}} O_i(t)$ denotes an average over the different runs of simulation, i.e., an average over the different time evolutions considering different set of random numbers.

This coefficient ranges from 0 to 1 and measures the ratio: (expected variation)/(total variation), so that the bigger the $r$, the better the linear fit of the data in log-scale. When the system is out of criticality, there is no power law and $r \approx 0$. However, at criticality ($y = y_c$ and $p = p_c$) or close to it, it is expected that $\rho(t)$ possesses a power law behavior given, for instance, by Eq. [7] and $r$ approaches to 1.
Therefore, we perform nonequilibrium MC simulations for each pair $y_i = i\Delta$ and $p_j = j\Delta$, with $i, j = 0, \ldots, n$ and $n = 1/\Delta$, in order to obtain color maps for the coefficient of determination as function of each pair $(y, p)$. Such maps are able to show the existence (or not) of phase transitions when diffusion of O atoms and CO molecules are allowed. The pair of critical values $(y_c, p_c)$ corresponds to $(y^{\text{opt}}, p^{\text{opt}}) = \arg\max_{y \in [0,1], p \in [0,1]}\{r\}$. A similar procedure has been used by the authors to study the effects of mobility on diluted lattices in an epidemic model [16]. In that work, they showed that mobility influences the immunization rates in such a way that the greater the mobility, the bigger the immunization rate.

It is important to mention that this technique can also be extended to study the weak first-order phase transitions [39], since these transitions possess long correlation lengths and small discontinuities and therefore behave similarly to second-order phase transitions [47] [48]. It has been conjectured that near a weak first-order transition there exist two pseudo-critical points: one point is just below (lower) the first-order phase transition point, and the other one is just above (upper) it. These pseudo-critical points are known as spinodal points [47].

### IV. RESULTS

In this work, we perform nonequilibrium MC simulations in order to obtain color maps for the phase transitions of the ZGB model with diffusion of O atoms and CO molecules adsorbed on the lattice. The results of our simulations are obtained by considering the coefficient of determination given by Eq. [9]. As stressed at the end of Sec. [1] we proposed two different approaches for each trial: Algorithm I, which considers that only one process (adsorption or diffusion) can occur in a given trial, and the Algorithm II in which both adsorption and diffusion processes are able to happen simultaneously.

In order to have a clue of the phase transitions of the model without spending too much computational time, we first performed rough simulations to be able to scan the entire space of parameters $y$ and $p$, i.e., $0 \leq y \leq 1$ and $0 \leq p \leq 1$, and construct complete color maps for the model. With these results in hand, we focused our attention in some regions of the color map where the transitions occur and refined our simulations, improving the accuracy of the results. In this study, we consider $L = 80$ and the parameters used in each stage are resumed in Table I.

Table I. Stages of simulation to obtain critical parameters with coefficient of determination.

| Stage                  | window | $N_{MC}$ | $N_{run}$ |
|------------------------|--------|----------|----------|
| 1 - Rough simulations  | $\Delta y = \Delta p = 0.005$ | 200 | 1000 |
| 2 - Refined simulations| $\Delta y = \Delta p = 0.001$ | 500 | 5000 |

Following, we present our main results obtained from the Algorithm I and Algorithm II.

#### A. Algorithm I - Diffusion process “XOR” adsorption process

In Fig. 1 (a) we show the color map which represents the possible regions of phase transitions of the ZGB model with diffusion. As can be seen, there are two regions that deserve more attention whereas their points $(y, p)$ are candidates to the continuous and discontinuous phase transition points, i.e., $r \equiv 1$. The first one is around the continuous phase transition of the original ZGB model ($y \equiv 0.3875$ and $p = 0$), and the second one is close to $y \equiv 0.525$ (the discontinuous phase transition point of the original ZGB model) and $p$ ranges from 0 to 1. At the top of this figure ($p \equiv 1$), there is a third region: a yellow horizontal strip that ranges from $0 \leq y \leq 1$. This region means that, in the most of cases, only the diffusion is allowed since $p \equiv 1$ and, although...
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$r \equiv 1$, the points in this region are not phase transition points as in the first two regions.

These “fake” phase transition points present exponent $\lambda \leq 0$ as suggested by Fig. 1(b), which shows the values of exponent $\lambda$ for the same ranges of $y$ and $p$. Differently from the “fake” points of the horizontal strip, the discontinuous phase transition (candidate) points along the vertical strip in Fig. 1(a) present $\lambda \equiv 2$ as again can be observed in Fig. 1(b). Such behavior includes the known $(y, p) \equiv (0.525, 0)$, which reinforces our confidence that diffusion transforms this point into an entire line of discontinuous phase transition points.

Moreover, the positivity for the exponents of these discontinuous phase transition points seems to be a good indicator to separate them from the continuous phase transition points since the last ones present negative exponents $\lambda$, that can be verified by taking the elliptical yellow region around $y \equiv 0.3875$ (continuous phase transition points) in Fig. 1(a) and their corresponding exponents in Fig. 1(b).

So, by looking into the Figs. 1(a) and (b), we are able to conclude that the diffusion eliminates the continuous phase transition and moves the discontinuous phase transition toward higher values of $y$. With these results in hand, we simulate the following two regions (refined simulations):

1. **Region 1**: $0.15 \leq y \leq 0.45$ and $0 \leq p \leq 0.15$, and
2. **Region 2**: $0.50 \leq y \leq 0.70$ and $0 \leq p \leq 1.00$.

Figure 2(a) shows the region 1 and 2(b) shows the region 2, using the parameters presented in the second line of Table I. From Fig. 2(a), one can see that $r$ is higher for smaller values of $p$ meaning that the continuous phase transition of the original ZGB model is destroyed for $p > 0$. Details about elliptical region near of expected critical point $y \equiv 0.3875$ and $p = 0$ can be observed. On the other hand, the discontinuous phase transition remains even for $p > 0$, as can be observed in Fig. 2(b).

In Fig. 3 we show the results from a simple procedure in which for each value of $y$, we span all different values of $p$, considering the region 1: 3(a) and the region 2: 3(b), and we plot $y \times p$ only for the points corresponding to the highest value of $r$ found by the procedure. We can observe that Fig. 3(a) indicates that only for values really low of $p$ (yellow points) we have candidates to continuous transition points, suggesting that the diffusion does not change the continuous transition point of the original ZGB model. On the other hand, Fig. 3(b) shows that a notorious line of discontinuous transition points are created.

**B. Algorithm II - Diffusion process “OR” adsorption process**

Finally, we performed simulations following the Algorithm II in which both adsorption and diffusion processes can occur in the same trial, i.e., diffusion does not exclude the possibility of adsorption. Thus, we carried out similar simulations and obtained plots as those shown previously in the Figs. 1, 2, and 3. The results obtained by considering the Algorithm II are collected and presented in Fig. 4.

In Fig. 4 the plots (a) and (b) correspond to the plots (a) and (b) of Fig. 2 respectively, the plots (c) and (d) correspond to the plots (a) and (b) of Fig. 4 respectively, and finally, the plots (e) and (f) correspond to the plots (a) and (b) of Fig. 3.

Exactly as shown for the Algorithm I, the continuous phase transition is destroyed for $p > 0$ and the discontinuous phase transition is maintained even for large values of $p$. In fact, it is important to notice that the discontinuous phase transition points remain practically the same for $0 \leq p \leq 1$ as can be observed in Fig. 4(a) which shows the coefficient of determination $r$. This behavior is corroborated by the value of the exponent $\lambda$ according
Figure 3. Plots obtained through a simple procedure in which for each value of \( y \), we look for a value of \( p \) that maximizes \( r \) for the region 1 (a) and the region 2 (b). The points correspond to the highest values of \( r \) found by the procedure.

to Fig. 4 (b). There is a small variation as suggested by the refined simulations of the region of discontinuous phase transition considered in Fig. 4 (d) but very different from Fig. 2 (b) which shows a strong curvature to the right side. We observe that the “fake” right discontinuous points disappear since diffusion and adsorption can occur simultaneously. However, regardless of the algorithm, Figs. 2 (b) and 4 (d) indicate that there exists a line of discontinuous phase transition for the ZGB model with diffusion. In addition, Figs. 2 (a) and 4 (c) are very similar and show that the diffusion eliminates the continuous phase transition of the original ZGB model.

The plot 4 (e) shows that highest values of the coefficient of determination are obtained only at the vicinity of the critical point of the original ZGB model, i.e., the diffusion destroys the continuous phase transition, as addressed before. However, it is important to notice that power laws consistent with continuous phase transition points are obtained for \( p_{\text{max}} \approx 0.08 \). And finally, 4 (f) shows that highest coefficient of determination suggests that the discontinuous phase transition points present small variations, \( 0.52 < y < 0.54 \), for \( 0 \leq p \leq 1 \) which is close to the discontinuous phase transition point of the original ZGB model, \( y = 0.525 \) and \( p = 0 \).

V. CONCLUSIONS

In this work, we studied the effects of the spatial diffusion on the phase transitions of the Ziff-Gulari-Barshad (ZGB) model by using an alternative method that optimizes the coefficient of determination in order to localize the critical parameters of the continuous phase transition point and to obtain an estimate of the upper spinodal point (one of the pseudo critical points of the model) of the weak discontinuous phase transition point.

Our results show that critical behavior is strongly changed by introducing the diffusion of the \( O \) atoms and \( CO \) molecules adsorbed on the lattice, leading to the extinction of the criticality even for small values of \( p \). On the other hand, we have an extension of discontinuous phase transition points for all values of the diffusion rates indicating that there exists a line of discontinuous transition points. For the Algorithm I, this line has a small curvature to the right and “fake” discontinuous transition points appear when \( p \rightarrow 1 \). For the Algorithm II these points are eliminated whereas both diffusion and adsorption processes are able to occur simultaneously. In addition, all points on the line of discontinuous phase transition obtained with the Algorithm II are close to the transition point of the original ZGB model.

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[1] R.M. Ziff, E. Gulari, and Y. Barshad, Phys. Rev. Lett. **56**, 2553 (1986).
[2] P. Meakin and D.J. Scalapino, J. Chem. Phys. **87**, 731 (1987).
[3] R. Dickman, Phys. Rev. A **34**, 4246 (1986).
[4] P. Fischer and U.M. Titulaer, Surf. Sci. **221**, 409 (1989).
[5] G.C. Bond, *Catalysis: Principles and Applications* (Clarendon, Oxford, 1987).
[6] V.P.Z. Zhdanov and B. Kazemo, Surf. Sci. Rep. **20**, 113 (1994).
[7] J. Marro and R. Dickman, *Nonequilibrium Phase Transitions in Lattice Models* (Cambridge University Press,
Figure 4. Here we used the algorithm II to obtain plots as those obtained through the Algorithm I. The plots (a) and (b) correspond to the plots (a) and (b) of Fig. 1 respectively. The plots (c) and (d) correspond to the plots (a) and (b) of Fig. 2 respectively, and finally, the plots (e) and (f) correspond to the plots (a) and (b) of Fig. 3.

[8] A. Golchet and J.M. White, J. Catal. 53, 266 (1978).
[9] T. Matsushima, H. Hashimoto, and I. Toyoshima, J. Catal. 58, 303 (1979).
[10] M. Ehsasi, M. Matloch, J.H. Block, K. Christmann, F.S. Rys, and W. Hirschwald, J. Chem. Phys. 91, 4949 (1989).
[11] K. Christmann, Introduction to Surface Physical Chemistry (Steinkopff Verlag, Darmstadt, 1991), pp. 1274.
[12] J.H. Block, M. Ehsasi, and V. Gorodetskii, Prog. Surf. Sci. 42, 143 (1993).
[13] H.K. Janssen, B. Schaub, and B. Schmittmann, Z. Phys. B: Condens. Matter 73, 539 (1989).
[14] G. Grinstein, Z.-W. Lai, and D.A. Browne, Phys. Rev. A 40, 4820 (1989).
[15] M. Dumont, P. Dufour, B. Sente, and R. Dagonnier, J. Catal. 122, 95 (1990).
[16] E.V. Albano, Appl. Phys. A 54, 2159 (1992).
[17] T. Tomé and R. Dickman, Phys. Rev. E 47, 948 (1993).
[18] H.P. Kaukonen and R.M. Nieminen, J. Chem. Phys. 91, 4380 (1989).
[19] I. Jensen and H. Fogedby, Phys. Rev. A 42, 1969 (1990).
[20] G.M. Buendia, E. Machado, and P.A. Rikvold, J. Chem. Phys. 131, 184704 (2009).
[21] B.C.S. Grandi and W. Figueiredo, Phys. Rev. E 65, 036135 (2002).
[22] G.L. Hoenicke and W. Figueiredo, Phys. Rev. E 62, 6216 (2000).
[23] G. M. Buendía and P.A. Rikvold, Phys. Rev. E 85, 031143 (2012).
[24] G. M. Buendía and P.A. Rikvold, Phys. Rev. E 88, 012132 (2013).
[25] G.M. Buendía, P.A. Rikvold, Phys. A 424, 217 (2015).
[26] G.L. Hoenicke, M.F. de Andrade, and W. Figueiredo, J. Chem. Phys. 141, 074709 (2014).
[27] J. Satulovsky and E.V. Albano, J. Chem. Phys. 97, 9440 (1992).
[28] E.V. Albano, Surf. Sci. 235, 351 (1990).
[29] B.J. Brosilow, E. Gulari, and R.M. Ziff, J. Chem. Phys. 98, 674 (1993).
[30] K. S. Trivedi, Probability and Statistics with Realiability, Queuing, and Computer Science and Applications, 2nd ed. (John Wiley and Sons, Chichester, 2002).
[31] R. da Silva, J.R. Drugowich de Felício, A.S. Martinez, Phys. Rev. E 85, 066707 (2012).
[32] R. da Silva, N. Alves Jr., J.R. Drugowich de Felício, Phys. Rev. E 87, 012131 (2013).
[33] R. da Silva, H.A. Fernandes, J.R. Drugowich de Felício, W. Figueiredo, Comput. Phys. Commun. 184, 2371 (2013).
[34] R. da Silva, H.A. Fernandes, J.R. Drugowich de Felício, Phys. Rev. E 90, 042101 (2014).
[35] R. da Silva, H.A. Fernandes, J. Stat. Mech. P06011 (2015).
[36] H.A. Fernandes, R. da Silva, E.D. Santos, P.F. Gomes, and E. Arashiro, Phys. Rev. E 94, 022129 (2016).
[37] W. Evans and M. S. Miesch, Phys. Rev. Lett. 66, 833 (1991).
[38] E.V. Albano, Chem. Rev. 3, 389 (1996).
[39] C.A. Voigt, R.M. Ziff, Phys. Rev. E 56 R6241 (1997).
[40] R.M. Ziff and B.J. Brosilow, Phys. Rev. A, 46 4630 (1992).
[41] R. da Silva, N.A. Alves and J.R. Drugowich de Felício, Phys. Lett. A 298, 325 (2002).
[42] H.A. Fernandes, Roberto da Silva, and J.R. Drugowich de Felício, J. Stat. Mech.: Theor. Exp., P10002 (2006).
[43] R. da Silva, J. R. Drugowich de Felício, A. S. Martinez, Phys. Rev. E, Statistical, 85, 066707 (2012).
[44] R. da Silva, R. Dickman, and J.R. Drugowich de Felício, Phys. Rev. E 70, 067701 (2004).
[45] P. Grassberger and Y. Zhang, Physica A 224, 169 (1996).
[46] R. da Silva and H.A. Fernandes, J. Stat. Mech. P06011 (2015).
[47] L. Schulke and B. Zheng, Phys. Rev. E 62, 7482-7485 (2000).
[48] E. Albano, Physics Letters A 288, 73–78 (2001).