Cluster-approximation mean-field theory of a class of cellular automaton models

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A cluster-approximation mean-field scheme, which may be used to describe some cellular automaton (CA) models, is introduced based on analyzing the evolution of cluster states. In this scheme the description of microscopic processes is exact within a cluster, and approximate for the interaction between clusters and the environment. The approach to building the theory is illustrated by a surface-reaction-like CA model very similar to the model of Ziff, Gulari, and Barshad. A set of equations of motion concerning the evolution of microscopic cluster states is derived, and some results from these equations are given.
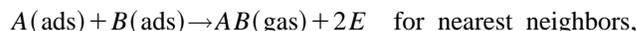[S1063-651X(99)05105-3]

Nonequilibrium dynamical systems may exhibit complicated behavior, including the formation of dissipative structures, oscillations, and kinetic phase transitions [1]. Because of the lack of a general theory, one has to adopt simple models (which take into account the essential features of the phenomena) to investigate such systems. Cellular automata (CA) serve as such simple models and have been used to investigate a variety of physical, chemical, and biological systems [2]. CA models describe a universe consisting of many discrete ''cells'' (lattice sites). Each site is endowed with a finite number of states, and all the sites update their states simultaneously at one time step according to a uniform local rule. Since spatial correlation is usually introduced in CA models, one would not expect the traditional mean-field theory to describe them correctly. In this paper we describe a cluster-approximation mean-field theory for a class of CA models. The steps to building the theory are outlined as follows. (a) For a general lattice with freedom parameter N, take a cluster with $N+1$ (or more) sites as an elementary unit, and make clear all its possible states. (b) Write down the cluster evolution rules according to a given CA local rule (the key step). (c) Write down the evolution equations concerning the probabilities of cluster states according to the cluster evolution rules and derive the corresponding master equations. (d) Perform calculations and analyses using these equations. We will illustrate our approaches by using a surface-reaction-like CA model. This model, though simple, may exhibit both first- and second-order kinetic phase transitions and thus is of interest in physics.

The model we use is very similar to that proposed by Ziff, Gulari, and Barshad (ZGB) [3]. The ZGB model has been proposed to mimic a monomer-dimer (A-B_2) reaction on a proper catalyst surface. The surface is modeled as a square lattice, and reactions proceed according to the following scheme:

$$A(\text{gas}) + E \rightarrow A(\text{ads}) \quad \text{with probability } X_A,$$

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$$B_2(\text{gas}) + 2E \rightarrow 2B(\text{ads}) \qquad \text{for nearest-neighbor } E,$$

$$\text{with probability } 1 - X_A,$$

$$A(\text{ads}) + B(\text{ads}) \rightarrow AB(\text{gas}) + 2E \quad \text{for nearest neighbors,}$$

where (gas) denotes the gas-phase species, (ads) denotes the adsorbed species, and an empty site on the lattice is denoted by E. This model has been thoroughly investigated by Monte Carlo (MC) simulations [3,4], and interesting behaviors are observed including the first- and second-order phase transitions between the steady reactive phase and A- and B-saturated phases. Noted that such a simple model cannot represent the complex physical and chemical processes occurring in even the most simple catalyst systems studied in the laboratory. It interests us because it provides a simple example of kinetic phase transitions of both first and second order, and such behaviors are of importance in many of areas [5].

In the following sections, we first give a CA version of ZGB model reaction on a general lattice, and then apply the cluster-approximation mean-field theory to this model. After the corresponding master equations are derived, we consider the average coverage fractions of the surface reactants as functions of X_A, and we give the phase diagrams for a triangular, square, and hexagonal lattice. Finally, some remarks are made.

CA VERSION OF THE ZGB MODEL

The present version is similar to that proposed by Chopard and Droz [6] but in a more general way. We consider a general lattice on which each site has N nearest neighbors. For a regular lattice, N has values of 2, 3, 4, or 6 for a linear, hexagonal, square, or triangular lattice, respectively (here we define the hexagonal and triangular lattice as the structures shown in Fig. 1). Above the lattice are the mixture gas phase molecules A and B_2 with concentrations X_A and $X_B = 1 - X_A$, respectively. Each lattice site may be in one of the following three states: A, B, and E (here we call them site states), meaning A-occupied, B-occupied, and empty state, respectively. All the site states update themselves simultaneously at one evolution step according to the following local rules. (i) An E transforms into A with probability X_A, or a conditional occupied state C with $1 - X_A$. This C immediately becomes B in the case of another C being
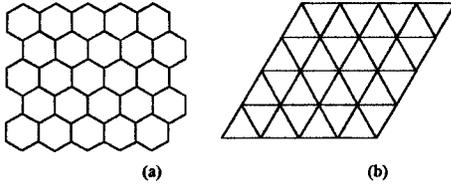
FIG. 1. The structures of hexagonal (a) and triangular (b) lattice defined in this paper.

FIG. 2. Example of degeneration: for a square lattice, a cluster state A-$\{3E,0A,1B\}$ contains four configurations.

found at its nearest-neighbor sites, otherwise it becomes E. (ii) An A (or B) transforms into E when there is at least one B (or A) at its nearest neighbors, otherwise it remains invariable. Note that in this model C is a fictitious state describing the impingement of B_2 on the lattice, and the reaction processes are assumed to be Langmuir-Hinshelwood-type.

CLUSTER STATES

We now take an $(N+1)$ site (a center site with N nearest neighbors) cluster as an elementary unit. Each cluster on the lattice may be in one of 3^{N+1} configurations (here 3 represents the number of different site states). We assume that the processes involved are equivalent in all directions. Thus these configurations degenerate to M (its value is given below) different cluster states, each distinguished from the others by its central site (denoted by X, here $X = E$, A, or B) and by the occupation number i, j, and k of E, A, and B states on its nearest-neighbor sites (denoted by $\{iE,jA,kB\}$, here $i=0,1,\ldots,N$, $j=0,1,\ldots,N-i$, and $k=N-i-j$). It is easy to see that the number of cluster states has the value

$$M=3\sum_{i=0}^{N}(N+1-i)=\tfrac{3}{2}(N+1)(N+2) \qquad (1)$$

and a cluster state, which is denoted by X-$\{iE,jA,kB\}$, contains $N!/i!j!k!$ different, but equivalent, configurations. Figure 2 shows an example of degeneration for $N=4$, $i=3$, $j=0$, and $k=1$.
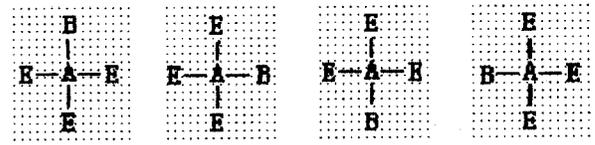
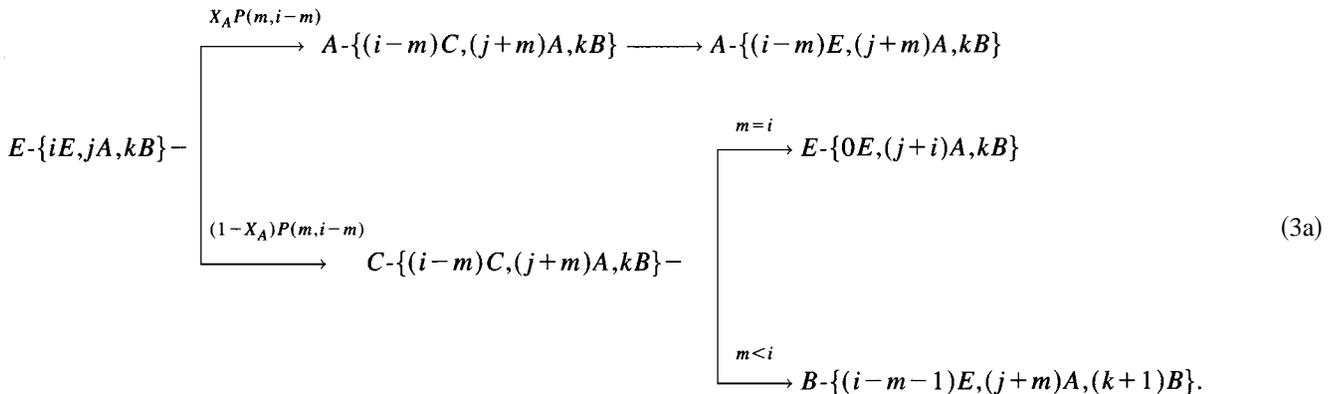## CLUSTER EVOLUTION RULES

It is necessary to distinguish two sorts of processes occurring in the evolution of a cluster. (i) The first are the processes inside a cluster, including the adsorption in an E cluster and the reaction between the central site and one of its nearest neighbors in an A or B cluster. Such processes may be completely followed and described exactly. (ii) The second are the interactions between a cluster and the environment, including the reactions of a cluster with the sites around it and the adsorption in an A or B cluster, which may be treated in a mean-field way. In the following we ignore, for simplicity, the later processes in formulating the cluster evolution rules, i.e., the clusters are regarded as isolated ones.

(i) *Adsorption.* Adsorption processes only occur in an E-$\{iE,jA,kB\}$ state. The central E transforms into A with probability X_A and into C with $1-X_A$ while m of the i nearest-neighbor E's transform into A's together with the remaining $i-m$ E's transforming into C's with probability

$$P(m,i-m)=\frac{i!}{m!(i-m)!}X_A^m(1-X_A)^{i-m}, \qquad (2)$$

where $m=0,1,\ldots,i$ and the normalization condition $\Sigma_{m=0}^{i}P(m,i-m)=1$ is maintained. If the transformed central site is A, its nearest-neighbor C sites immediately transform back into E's, while if the transformed central site is C, it becomes E for $m=i$ (no C site being found in its nearest neighbors), or becomes B for $m<i$. In the latter case one of the nearest-neighbor C's also becomes B and the remaining $i-m-1$ C's become E's. The rule described above may be summarized as follows:

$$
\begin{array}{l}
\xrightarrow{X_A P(m,i-m)} A\text{-}\{(i-m)C,(j+m)A,kB\} \longrightarrow A\text{-}\{(i-m)E,(j+m)A,kB\} \\[2em]
E\text{-}\{iE,jA,kB\}- \\[2em]
\qquad \xrightarrow{(1-X_A)P(m,i-m)} C\text{-}\{(i-m)C,(j+m)A,kB\}-
\end{array}
$$

$$
\begin{array}{l}
\xrightarrow{m=i} E\text{-}\{0E,(j+i)A,kB\} \\[2em]
\xrightarrow{m<i} B\text{-}\{(i-m-1)E,(j+m)A,(k+1)B\}.
\end{array}
$$

(3a)

(ii) *Reaction.* Reaction processes occur in A (and B) clusters in cases in which at least one nearest-neighbor B (and A) is found. In each of the reaction events, the central A (or B) together with one of its nearest-neighbor B (or A) becomes E states. The rules may be formulated as

$$A\text{-}\{iE,jA,kB\} \xrightarrow{k>0} E\text{-}\{(i+1)E,jA,(k-1)B\}, \quad (3b)$$

$$B\text{-}\{iE,jA,kB\} \xrightarrow{j>0} E\text{-}\{(i+1)E,(j-1)A,kB\}. \quad (3c)$$

EQUATIONS OF MOTION: EVOLUTION OF CLUSTER STATES

Let $x(i,j,k)$ denote the probability of finding a cluster state $X\text{-}\{iE,jA,kB\}$ on the lattice, and let $x^{\pm}(i,j,k)$ denote the variances (where $x=a$, b, and e corresponds to $X=A$, B, and E, and $+/-$ denotes the increase/decrease). From the evolution rules (3a)–(3c), one can easily write out the evolution equations in terms of probabilities at one evolution step:

$$a^{+}(i-m,j+m,k)=X_A P(m,i-m)e(i,j,k), \quad (4a)$$

$$b^{+}(i-m-1,j+m,k+1)=(1-X_A)P(m,i-m)e(i,j,k), \quad (4b)$$

$$e^{+}(0,i+j,k)=(1-X_A)P(i,0)e(i,j,k), \quad (4c)$$

$$e^{-}(i,j,k)=-e(i,j,k), \quad (4d)$$

$$e^{+}(i+1,j,k-1)=a(i,j,k), \quad (4e)$$

$$e^{+}(i+1,j-1,k)=b(i,j,k), \quad (4f)$$

$$a^{-}(i,j,k)=-\alpha(i,j,k), \quad (4g)$$

$$b^{-}(i,j,k)=-\beta(i,j,k), \quad (4h)$$

where the functions $\alpha(i,j,k)$ and $\beta(i,j,k)$ are defined, according to Eqs. (3b) and (3c), as

$$\alpha(i,j,k)=\begin{cases} a(i,j,k) & \text{for } k>0, \\ 0 & \text{for } k=0, \end{cases} \quad (5a)$$

$$\beta(i,j,k)=\begin{cases} b(i,j,k) & \text{for } j>0, \\ 0 & \text{for } j=0. \end{cases} \quad (5b)$$

After some operations of parameters rearranging and uniting the terms, Eqs. (4a)–(4h) may be systematized as follows:

$$a^{+}(i,j,k)=\sum_{m=0}^{j} X_A P(m,i)e(i+m,j-m,k), \quad (6a)$$

$$b^{+}(i,j,k)=\sum_{m=0}^{j} (1-X_A)P(m,i+1) \\ \times e(i+m+1,j-m,k-1), \quad (6b)$$

$$e^{+}(0,j,k)=\sum_{m=0}^{j} (1-X_A)P(m,0)e(m,j-m,k), \quad (6c)$$

$$e^{+}(i,j,k)=a(i-1,j,k+1)+b(i-1,j+1,k), \quad (6d)$$

$$e^{-}(i,j,k)=-e(i,j,k), \quad (6e)$$

$$a^{-}(i,j,k)=-\alpha(i,j,k), \quad (6f)$$

$$b^{-}(i,j,k)=-\beta(i,j,k), \quad (6g)$$

where $P(m,i)=[(m+i)!/m!i!]X_A^m(1-X_A)^i$, $P(m,i+1)=[(m+i+1)!/m!(i+1)!]X_A^m(1-X_A)^{i+1}$, and $P(m,0)=X_A^m$. From the above equations one can easily construct the equations of motion concerning the evolution of cluster states as follows:

$$\frac{d}{dt}a(i,j,k)=\sum_{m=0}^{j} X_A P(m,i)e(i+m,j-m,k)-\alpha(i,j,k), \quad (7a)$$

$$\frac{d}{dt}b(i,j,k)=\sum_{m=0}^{j} (1-X_A)P(m,i+1) \\ \times e(i+m+1,j-m,k-1)-\beta(i,j,k), \quad (7b)$$

$$\frac{d}{dt}e(i,j,k)=\sum_{m=0}^{j} (1-X_A)P(m,0)e(m,j-m,k) \\ +a(i-1,j,k+1)+b(i-1,j+1,k)-e(i,j,k), \quad (7c)$$

which are known as master equations [7]. Note that Eqs. (7a)–(7c) contain $M=\frac{3}{2}(N+1)(N+2)$ equations for different i and j, and only $M-1$ of them are independent, considering the normalization condition

$$\sum_{i=0}^{N}\sum_{j=0}^{N-i} [a(i,j,k)+b(i,j,k)+e(i,j,k)]=1. \quad (7d)$$

Defining a state vector $S(t)$, which may be represented as a matrix of M dimension in probability space, and an evolution operator W, a matrix of $M\times M$ dimension, Eqs. (7a)–(7c) may be formed as

$$\frac{d}{dt}S(t)=WS(t) \quad (8a)$$

or in a recursive form as

$$S(t)=TS(t-1)=T^2S(t-2)=\cdots=T^tS(0), \quad (8b)$$

where $T=I+W$ (here I represents an identity matrix), known as the transition matrix. In principle this matrix may give all the information about the evolution of cluster states for a given CA model. In the following sections we only consider the average coverage fractions of surface reactants, which may be obtained by performing the average over all the cluster states.

EQUATIONS OF MOTION: EVOLUTION OF AVERAGE COVERAGES

Let θ_X denote the average coverage of X states on the lattice and θ_{XY} denote that of nearest-neighbor XY pairs. The normalization conditions $\Sigma_X \theta_X = 1$ and $\Sigma_X(\theta_{XX} + \frac{1}{2}\Sigma_{Y\neq X}\theta_{XY}) = 1$ give the relation between site and pair coverage as

$$\theta_X = \theta_{XX} + \frac{1}{2}\sum_{Y\neq X}\theta_{XY}, \tag{9}$$

thus in an X cluster the probability of finding an XX pair is

$$x_X = \frac{\theta_{XX}}{\theta_X} \tag{10a}$$

while that of finding an XY pair $(X\neq Y)$ is

$$x_Y = \frac{\theta_{XY}}{2\theta_X}, \tag{10b}$$

where $x = e$, a, and b, corresponding to E, A, and B clusters, and such quantities are normalized: $x_X + \Sigma_{Y(\neq X)}x_Y = 1$.

Defining quantities as above, the probability of finding a cluster state X-$\{iE, jA, kB\}$ on the lattice in terms of site and pair probabilities may be formulated as

$$x(i,j,k) = \frac{N!}{i!j!k!}\theta_X x_E^i x_A^j x_B^k \tag{11}$$

with the condition $\Sigma_{i=0}^N \Sigma_{j=0}^{N-i} x(i,j,k) = \theta_X$.

Starting from the cluster evolution equations (4a)–(4h), and summing up the variances of each pair coverage over all cluster states, it is not difficult to deduce the equations of motion concerning the evolution of each pair average coverage. For example, the increase of θ_{AA} may be obtained from Eq. (4a):

$$\theta_{AA}^+ = \sum_{i=0}^{N}\sum_{j=0}^{N-i}\sum_{m=0}^{i}\frac{j+m}{N}a^+(i-m,j+m,k)$$

$$= \frac{1}{2}\theta_{AE}X_A + \theta_{EE}X_A^2,$$

while its decrease from Eq. (4g) is

$$\theta_{AA}^- = \sum_{i=0}^{N}\sum_{j=0}^{N-i}\frac{j}{N}a^-(i,j,k) = -\theta_{AA}[1-(1-a_B)^{N-1}]$$

and thus

$$\frac{d\theta_{AA}}{dt} = \theta_{AA}^+ + \theta_{AA}^- = \frac{1}{2}\theta_{AE}X_A + \theta_{EE}X_A^2$$

$$- \theta_{AA}[1-(1-a_B)^{N-1}]. \tag{12a}$$

Constructed in the similar way, and defining $u \equiv 1 - e_E(1-X_A)$, $v \equiv 1 - a_B$, and $w \equiv 1 - b_A$, the other equations are obtained as follows:

$$\frac{d\theta_{BB}}{dt} = \frac{1}{2}\theta_{BE}(1-X_A)(1-u^{N-1})$$

$$+ \frac{1}{N}\theta_E(1-X_A)(1-u^N) - \theta_{BB}(1-w^{N-1}), \tag{12b}$$

$$\frac{d\theta_{EE}}{dt} = \frac{1}{2}\theta_{AE}(1-v^{N-1}) + \frac{1}{2}\theta_{BE}(1-w^{N-1})$$

$$+ \frac{1}{N}\theta_A(1-v^N) + \frac{1}{N}\theta_B(1-w^N) - \theta_{EE}, \tag{12c}$$
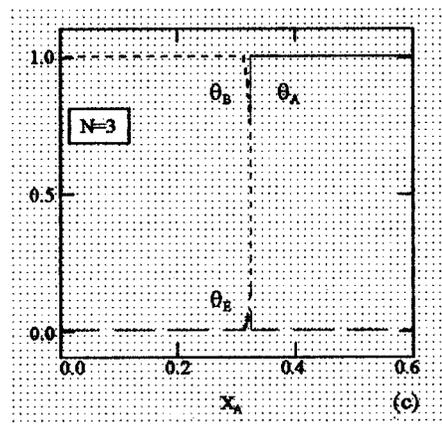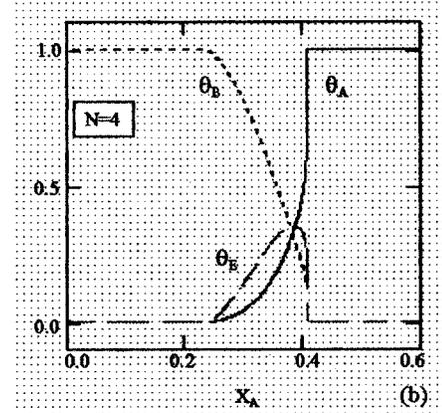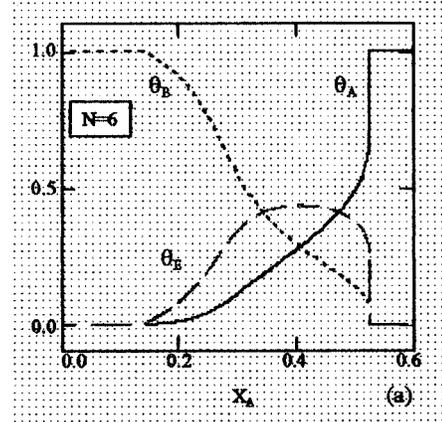

FIG. 3. Phase diagrams of the AB_2 model surface reaction on (a) triangular, (b) square, and (c) hexagonal lattices. The average coverages θ_A (——), θ_B (– – –), and θ_E (——) as functions of X_A.

TABLE I. The transition values and the dimer coverage at $X_A=0$ for different lattice freedom N.

Freedom number	Second-order transition value	First-order transition value	θ_B at $X_A=0$ (case 1)	θ_B at $X_A=0$ (case 2)
6	0.138 ± 0.002	0.5251 ± 0.0001	0.5833	0.8582
4	0.242 ± 0.002	0.4068 ± 0.0001	0.6250	0.8535
3	0.312 ± 0.002	0.3239 ± 0.0001	0.6667	0.8519
2			0.7500	0.8125

$$\frac{d\theta_{AB}}{dt} = \tfrac{1}{2}\theta_{BE}X_A + (\tfrac{1}{2}\theta_{AE} + \theta_{EE}X_A)$$

$$\times (1-X_A)(1-u^{N-1}) - \theta_{AB}, \qquad (12d)$$

$$\frac{d\theta_{AE}}{dt} = \theta_{EE}X_A(1-X_A)(1-u^{N-1}) + \tfrac{1}{2}\theta_{AE}(1-X_A)u^{N-1}$$

$$+ \tfrac{1}{2}\theta_{AB} + (\theta_{AA} + \tfrac{1}{2}\theta_{AE})(1-v^{N-1})$$

$$- \frac{1}{N}\theta_B(1-w^N) - \tfrac{1}{2}\theta_{AE}, \qquad (12e)$$

$$\theta_{BE} = 1 - \theta_{AA} - \theta_{BB} - \theta_{EE} - \theta_{AB} - \theta_{AE}, \qquad (12f)$$

where θ_X ($X=A$, B, or E), e_E, a_B, and b_A are determined by Eqs. (9), (10a), and (10b), respectively.

PHASE DIAGRAMS

The stable solutions of Eqs. (12a)–(12f) may be obtained by carrying out the numerical integration of these equations. Given values of N and X_A, the integration will lead to a steady state of a macrocosm in which the average coverages θ_A, θ_B, and θ_E never change. Figure 3 shows the coverages θ_A, θ_B, and θ_E as functions of X_A for different N, and Table I presents the transition values and the values of θ_B at the point $X_A=0$, in which all the integrations start from the initial values: $\theta_{EE}=1$ and $\theta_{AA}=\theta_{BB}=\theta_{AB}=\theta_{AE}=\theta_{BE}=0$.

For $N=6$ (triangular lattice), 4 (square), and 3 (hexagonal), there are three phases which are the B-saturated, A-saturated, and steady reactive phase. The transition between B-saturated and reactive phase is of second order (continuous), while that between the reactive and A-saturated phase is of first order (discontinuous), just as observed in MC [3,4] and CA [6,8] simulations. The reactive window decreases its width with N taking a lower value, in agreement with that observed in MC simulations for square and triangular lattices [4]. The transition values (the bounds of the reactive window) for different N are given in Table I.

It is a natural conclusion from Fig. 3 and Table I that for $N=2$ (linear lattice) the width of the reactive window decrease to zero (and to at least less than 0.012 for $N=3$). This conclusion is confirmed by our integration in which θ_E always vanishes for any value of X_A but zero.

RANDOM DIMER FILLING PROBLEM

The behavior at the point $X_A=0$ deserves further comment. In this case the model corresponds to the random dimer filling problem [9]. In the CA version of a surface-

reaction-like model, all processes will stop after one evolution step. Starting from the blank lattice [$e(N,0,0)=1$], the evolution rule may be formulated as

$$E\text{-}\{NE,0A,0B\} \rightarrow C\text{-}\{NC,0A,0B\} \rightarrow B\text{-}\{(N-1)C,0A,1B\}.$$
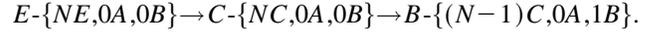
In the case of ignoring the interaction between clusters (case 1), as in the above text, all the nearest-neighbor C's become E [$B\text{-}\{(N-1)C,0A,1B\} \rightarrow B\text{-}\{(N-1)E,0A,1B\}$], and the coverage θ_B may be obtained as

$$\theta_B = \theta_{BB} + \tfrac{1}{2}\theta_{BE} = \frac{1}{N} + \frac{N-1}{2N} = \frac{N+1}{2N}. \qquad (13)$$

The values of θ_B for different N are given in Table I.

Better results may be obtained by considering the interaction of a cluster with the environment (case 2). In this case each nearest-neighbor C has a probability p_c for transforming into B, dependent upon the states of the outerlayer sites around it. Thus m of $N-1$ nearest-neighbor C's transforming into B together with the remaining ones becoming E [$B\text{-}\{(N-1)C,0A,1B\} \rightarrow B\text{-}\{(N-1-m)E,0A,(m+1)B\}$] has a probability

$$q(m,N-1-m) = \frac{(N-1)!}{m!(N-1-m)!} p_c^m (1-p_c)^{N-1-m}, \qquad (14)$$

where p_c is dependent on the dimension of lattice. For a linear lattice ($N=2$), each cluster has N ($=2$) outerlayer nearest-neighbor sites around it, and thus $p_c=\theta_C$, while for a two-dimensional lattice ($N>2$), each $(N+1)$-site cluster has $2N$ outerlayer nearest neighbors around it, and thus $p_c = 1-(1-\theta_C)^2$. Here $\theta_C = \tfrac{1}{2}\theta_{BC} = (N-1)/2N$.

By the same argument given in the preceding paragraphs, θ_B may be constructed as

$$\theta_B = \begin{cases} 1 - \tfrac{1}{8}\left(1-\dfrac{1}{N}\right)\left(1+\dfrac{1}{N}\right)^2 & \text{for } N>2, \\[2mm] 0.8125 & \text{for } N=2. \end{cases} \qquad (15)$$

The values are also given in Table I.

REMARKS

(i) *The Mean-field theory.* The simplest and most frequently used tool is the site-approximation approach, which ignores all the spatial correlations and local fluctuations, and thus is usually used to get a quick impression of the behaviors in a system, or to give an outlining explanation of some computer-simulated results. To describe a system more accurately, we need the cluster-approximation approach. Dick-

man has described a pair-approximation mean-field scheme [10] for the ZGB model surface reaction on a square lattice, based on analyzing the ''processes'' of the reaction. Our approach belongs to another type which is based on analyzing the evolution of ''lattice states.''

(ii) *The present scheme.* (a) The scheme consists of a general lattice upon which a CA model is formulated. The lattice freedom parameter N enters into the theory. This allows us to analyze the effect of geometric factors on the kinetics in a model dynamical system, when necessary. (b) As presented in the text, it is an easy-to-operate scheme. Once the cluster evolution rules are formulated according to a given CA model, the remaining derivations are quite distinct and simple. In particular, there is no difficulty when considering different types of lattices. (c) Because the scheme involves the evolution of lattice states rather than the special processes of dynamics, it has the advantage of being able to turn from one model to another without special difficulties. We will present further studies elsewhere.

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