Propagating waves in one-dimensional discrete networks of coupled units

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We investigate the behavior of discrete systems on a one-dimensional lattice composed of localized units interacting with each other through nonlocal, nonlinear reactive dynamics. In the presence of second-order and third-order steps coupling two or three neighboring sites, respectively, we observe, for appropriate initial conditions, the propagation of waves which subsist in the absence of mass transfer by diffusion. For the case of the third-order (bistable) model, a counterintuitive effect is also observed, whereby the homogeneously less stable state invades the more stable one under certain conditions. In the limit of a continuous space the dynamics of these networks is described by a generic evolution equation, from which some analytical predictions can be extracted. The relevance of this mode of information transmission in spatially extended systems of interest in physical chemistry and biology is discussed.

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I. INTRODUCTION

The origin and modeling of wave propagation in purely dissipative systems as opposed to systems possessing inertia encountered in mechanics, electromagnetism and fluid dynamics, has attracted wide interest and motivated a large amount of theoretical and experimental studies. Typically, these studies are concerned with the behavior of networks of localized nonlinear active units such as well-stirred chemical reactors [1–3], living cells [4–7], or individuals in an ecosystem [8–12] which are coupled in space by diffusive transport. In the continuous space limit the dynamics of such systems reduces to a set of reaction-diffusion equations. There exists an array of analytic and numerical tools, starting from the classical work of Kolmogorov, Petrovski, and Piskounov [13], allowing for a good understanding of the onset and of the essential quantitative properties of the wave fronts and related phenomena generated by these equations depending on the values of the parameters, the initial and the boundary conditions [9,14].

In this article we explore the behavior of discrete systems for which spatial communication between the constitutive elements of the network does not entirely rely on diffusion or any other classical mass transport. Reactive dynamics in such systems is not purely local, but involves the state of neighboring units as well. In opposition to the classical process of mass transport, the precise form of this new spatial coupling depends on the mechanistic details of the dynamical process considered and is thus expected to be nonlinear and system dependent. A typical example giving rise to a coupling of this kind is provided by reactions on low-dimensional supports encountered, for instance, in heterogeneous catalysis [15–24]. The behavior of these systems can often be mapped into a spinlike dynamics, for which there exists a rich literature from statistical physics, particularly in the context of phase transitions [25].

So far the role of this particular form of spatial coupling in the onset of nontrivial spatiotemporal dynamics has not been studied systematically. Our main objective will be to shed some light on the possible influence of such nonlocal reactive processes on the propagation of waves. To this end we compare three levels of description: the classical mass-action (MA) dynamics, the discrete, nonlocal (DNL) evolution laws, and the continuous space limit of the DNL rate equation, hereafter referred to as continuous nonlocal (CNL) dynamics. We focus on the case of one-dimensional, one-species models with interactions involving only first neighbors of each site, but the extension to more intricate systems is straightforward.

The general formulation is presented in Sec. II. Special emphasis is placed on the spatially continuous limit of the evolution equation (the CNL equation), from which some useful analytical results can be extracted. As a first illustration, a second-order Schlögl-Fisher model involving two neighboring sites of the network is studied in Sec. III. Since this system admits one stable and one unstable state in the homogeneous limit, one expects the propagation of waves for appropriate initial conditions. We show that the reactive coupling is equivalent to a nonlinear effective diffusion that modifies the shape and the velocity of the propagating front. Of special interest is the existence of propagation of waves in the total absence of diffusion. We next consider in Sec. IV a third-order model giving rise to bistability. The effects associated with nonlocal dynamics are here even more surprising, since the direction of propagation of the waves is reversed when diffusion is low. We give for this unexpected feature an analytical interpretation based on a perturbative development of the aforementioned CNL evolution equation. The main conclusions and the possible implications and further developments are summarized in Sec. V.

II. GENERAL FORMULATION

We consider in this work one-dimensional networks composed of a large number N of interacting units. The state of

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each of the localized units can be modified by r different elementary processes involving adjacent sites,

$$\sum_{\alpha}\sum_{j=-1}^{j=+1}\nu_{\alpha,\rho}(i+j)\mathrm{X}_{\alpha}(i+j) \overset{k_\rho}{\rightarrow} \sum_{\alpha}\sum_{j=-1}^{j=+1}\nu^{*}_{\alpha,\rho}(i+j)\mathrm{X}_{\alpha}(i+j)$$

$$\rho=1,\ldots,r,$$

$$\alpha=1,\ldots,n,$$

$$i=1,\ldots,N. \tag{1}$$

Here $X_\alpha(i)$ represents the population of species α in the unit i. The j's are the first neighbors of i and $\nu_{\alpha,\rho}(i+j)$, $\nu^{*}_{\alpha,\rho}(i+j)$ are the local stoichiometric coefficients of, respectively, reactant and product α for the elementary step considered. The evolution of the local state variable $c_\alpha(i,t)$ (such as, for example, the local concentration of X_α) at each site can be described by a differential-difference equation containing a nonlocal interaction term h_α and, if the elements are free to move on the lattice, an additional coupling by ordinary diffusion,

$$\frac{d}{dt}c_\alpha(i,t)=h_\alpha(\{c_\alpha(i,t)\},\{c_\alpha(i\pm1,t)\}) + \frac{\Gamma}{2}[c_\alpha(i+1,t)+c_\alpha(i-1,t)-2c_\alpha(i,t)], \tag{2}$$

where Γ is the hopping probability. The specific form of h_α describes how the state of the site i is modified by the different elementary processes. In the sequel it will be modeled by an extended, nonlocal mass-action law

$$h_\alpha(\{c_\alpha(i,t)\},\{c_\alpha(i\pm1,t)\}) = \sum_{\rho} k_\rho[\nu^{*}_{\alpha,\rho}(i)-\nu_{\alpha,\rho}(i)] \times\prod_{\alpha'}\prod_{j=-1}^{j=+1}[c_{\alpha'}(i+j,t)]^{\nu_{\alpha',\rho}(i+j)}. \tag{3}$$

For the sake of simplicity, we limit ourselves from now on to two-species models with conservation of the total concentration. There is, therefore, only one active species, the second one being related to the vacant sites of the lattice, but the analysis could be extended to more intricate schemes.

To obtain some analytic insight it will be useful to consider a continuous-space approximation of Eq. (2), taken by introducing the spatial coordinate $r=ia$, where a is the lattice parameter, i.e., the distance between two first neighbors, and supposing that this parameter can be taken small in comparison with the total size of the system or with the characteristic scale at which the concentration varies appreciably. Under these conditions, one can expand the local concentration in the form

$$c(r\pm a,t)\approx c(r,t)\pm a\nabla c(r,t)+\frac{a^2}{2}\nabla^2 c(r,t)+\cdots.$$

Keeping the terms up to the second order in a, one obtains an evolution equation of the form

$$\frac{\partial}{\partial t}c(r,t)=f(c(r,t))+g(c(r,t))[\nabla c(r,t)]^2 + D(c(r,t))\nabla^2 c(r,t) \tag{4}$$

referred to subsequently as the CNL evolution equation. To understand the meaning of this equation we recall the form of traditional evolution laws as deduced from the mean-field approximation,

$$\frac{\partial}{\partial t}c(r,t)=f(c(r,t))+D\nabla^2 c(r,t). \tag{5}$$

For the systems considered here [a single dependent variable $c(r,t)$] this evolution law can be derived from a potential functional

$$\frac{\partial}{\partial t}c(r,t)=-\frac{\delta}{\delta c(r)}\mathcal{F}[c(r,t)],$$

$$\mathcal{F}[c(r,t)]=\mathcal{U}[c(r,t)]-\int\frac{1}{2}D[\nabla c(r,t)]^2 dr,$$

where $\mathcal{U}[c(r,t)]=-\int f[c(r,t)]dc(r,t)$ is the kinetic potential, reducing near equilibrium to the product of a free energy function and an Onsager coefficient. In the case of multistability, the state with lowest $\mathcal{U}[c(r,t)]$ is the most stable state, and the other states are metastable. We clearly recognize in Eq. (4) corrections to the usual mean-field evolution laws (5). Comparing these equations, we note that they both comprise a local MA evolution law $f(c(r))$ and a diffusion term. This term is characterized by a diffusion coefficient D which is essentially constant in the mean-field equation, but concentration-dependent in Eq. (4), typically involving the sum of the traditional diffusion coefficient and of contributions arising from the nonlocal dynamics. Finally, the CNL equation displays in its right-hand side an extra dissipative term $g(c(r,t))[\nabla c(r,t)]^2$. A similar term appears in the deterministic limit of the KPZ equation [26]. There are however some substantial differences: the presence of a state dependent coefficient multiplying the Laplacian and gradient square terms and the scalar term reflecting a nontrivial local dynamics. Finally, note that contrary to the mean-field equation, the evolution law (4) cannot in general be derived from a potential.

Before switching to the analysis of specific classes of models, we compile some general conclusions about the continuous limit (4), in connection with wave propagation.

Using standard techniques, we introduce the change of variables $r \to r - vt$, where v is a constant velocity. Equation (4) then becomes

$$-vU'(z) = f(U(z)) + g(U(z))[U'(z)]^2 + D(U(z))U''(z), \tag{6}$$

where $U(z) = c(r - vt, t)$ and $'$ denotes derivative with respect to z. This equation can be mapped into a dynamical system involving the two variables $U(z) = c(r - vt, t)$ and $V(z) = U'(z)$, described by the following ordinary differential equations:

$$\begin{cases} U'(z) = V(z) \\ V'(z) = [-vV(z) - g(U(z))V(z)^2 \\ \qquad - f(U(z))]/D(U(z)). \end{cases} \tag{7}$$

Provided that $D(U(z)) \neq 0$, the linear stability of the steady-states $(U_{st}, V_{st}) = (c_i, 0)$, with $f(c_i) = 0$, can be easily tested, and to each state we may associate the two eigenvalues of the corresponding Jacobian matrix,

$$\omega_i = -\frac{v}{2D(c_i)} \pm \frac{1}{2}\sqrt{\frac{v^2}{D(c_i)^2} - 4\frac{f'(c_i)}{D(c_i)}}, \tag{8}$$

where $f'(c_i)$ is the first derivative of $f(U(z))$ with respect to $U(z)$, taken at $U(z) = c_i$. This quantity will prove useful in estimating the minimal velocity of waves between unstable and stable states, in comparison with the mean-field predictions where the diffusion coefficient has no dependence in c_i. Note that the linear stability of the fixed points does not involve explicitly the dissipative term $g(U(z))$.

In the following two sections we consider two prototypical systems in which unexpected behavior of front propagation is observed, and show how these phenomena are induced by the nonlocal dynamics.

III. WAVE FRONTS BETWEEN STABLE AND UNSTABLE STATES

We first investigate an irreversible discrete, two-species Schlögl-Fisher model described by the mechanism

$$X_2(i) + X_1(i \pm 1) \to X_1(i) + X_1(i \pm 1) \quad k_1, \tag{9}$$

$$X_1(i) \to X_2(i) \quad k_2, \tag{10}$$

$$X_1(i) + X_2(i \pm 1) \rightleftharpoons X_2(i) + X_1(i \pm 1) \quad \Gamma. \tag{11}$$

The first step describes an autocatalytic process producing X_1, the second one a simple decomposition, and the third step an exchange reaction. Following the conservation law introduced in Sec. II, X_1 and X_2 are here to be interpreted as, respectively, the population of sites of a lattice filled with reactant X_1 and the empty sites. In the terminology of surface reactions, e.g., Eq. (9) can be seen as a cooperative adsorption, Eq. (10) as a spontaneous desorption, and Eq. (11) as diffusion (random walk) induced mass transport. The corresponding local concentrations satisfy $c_1(i) = 1 - c_2(i)$,

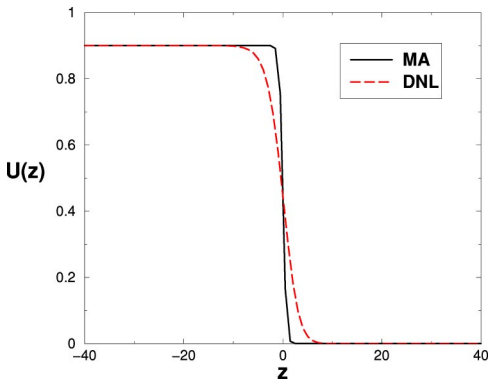

FIG. 1. Shape of the front obtained, respectively, from the discrete localized rate equation (MA) and the discrete nonlocal dynamics (DNL) for the Sclhögl-Fisher model. The spatial variable is $i - v_{\min}t$, i.e., we are in the comoving frame in a discrete network composed of 10 000 sites, with periodic boundaries. $k_1 = 1.0$, $k_2 = 0.1$, Γ is here 0.01. The initial condition is as described in Eqs. (14) and (15), and dimensionless units are used.

reducing the problem to a one-species model. The DNL equation corresponding to the mechanism reads

$$\frac{d}{dt}c(i) = \frac{k_1}{2}(1 - c(i))[c(i+1) + c(i-1)] - k_2 c(i) + \frac{\Gamma}{2}[c(i+1) + c(i-1) - 2c(i)] \tag{12}$$

$$= k_1 c(i)(1 - c(i)) - k_2 c(i) + \left[\frac{\Gamma}{2} + \frac{k_1}{2}(1 - c(i))\right]\Delta c(i), \tag{13}$$

where $c(i) = c_1(i)$ and $\Delta c(i)$ denotes the discretized Laplacian. The 1/2 factors before the autocatalytic and diffusion steps come from the fact that the nearest neighbor to the right or to the left contribute with equal probability. The form of this evolution law allows one to understand how the discreteness of the network, together with the nonlocal character of the reactive events, is indeed responsible for the appearance of a concentration-dependent diffusion coefficient in Eq. (4).

In the homogeneous limit, and as long as $k_1 > k_2$, Eq. (12) admits one stable steady state $(c_1 = (k_1 - k_2)/k_1)$ and one unstable steady state $(c_2 = 0)$. In the corresponding spatially extended system, if only the $\Gamma a^2/2$ term were present in the coefficient of the second derivative, one would obtain a wave propagating from left to right if the lattice is initially prepared so that

$$c(r,0) = c_1 \quad \text{as} \quad r \to -\infty, \tag{14}$$

$$c(r,0) = c_2 \quad \text{as} \quad r \to +\infty. \tag{15}$$

Moreover, we know that if the front between these two states is sharp enough at $t = 0$, the wave propagates with a given minimal velocity. Figure 1 depicts the composition profile as a result of the numerical solution of such a reduced form of Eq. (12) (full line) along with a numerical solution of the full

Eq. (12) itself (dashed lines) on a discrete lattice subject to an initial condition in the form of a Heaviside function. We see that the wave character of the solution subsists, but that the profile of the front is modified.

In order to assess the relative roles of classical diffusion and of discrete delocalized dynamics in the wave propagation, we resort to the continuous limit of Eq. (13) described by

$$\frac{\partial c}{\partial t} = k_1 c[1-c] - k_2 c + \left[\frac{\Gamma a^2}{2} + \frac{k_1 a^2}{2}(1-c)\right]\nabla^2 c. \tag{16}$$

Note the absence of the gradient square term expected to appear in the most general case [Eq. (4)]. In the two-dimensional phase space $(U(z),V(z))$ introduced in Sec. II, the dynamical system in which this equation reduces admits two fixed points: $(c_1,0)$ and $(0,0)$, whose stability is determined by

$$\omega_{c_1} = -\frac{v}{2D(c_1)} \pm \frac{1}{2}\sqrt{\frac{v^2}{D(c_1)^2} - 4\frac{f'(c_1)}{D(c_1)}},$$

$$\omega_0 = -\frac{v}{2D(0)} \pm \frac{1}{2}\sqrt{\frac{v^2}{D(0)^2} - 4\frac{f'(0)}{D(0)}}.$$

Since $f'(c_1)<0$ and $D(c_1)>0$, the corresponding state is a saddle point. The nature of the other fixed point depends on the sign of Δ (the discriminant inside the square root) and since $f'(0)>0$ we have a stable node if $\Delta \geqslant 0$, and a stable focus otherwise. There are thus heteroclinic trajectories linking the two steady states in this phase space. We note that $U(z)$ must be positive so that the system cannot "spiral down" to (0,0), and thus that Δ should in fact be nonnegative. This condition gives us the minimal velocity

$$v_{\min}^{\mathrm{CNL}} = 2a\sqrt{(k_1-k_2)\left[\frac{\Gamma+k_1}{2}\right]}. \tag{17}$$

Note that in classical mean field, MA rate equations the diffusion coefficient is simply $\Gamma a^2/2$, leading to

$$v_{\min}^{\mathrm{MA}} = 2a\sqrt{(k_1-k_2)\frac{\Gamma}{2}}. \tag{18}$$

A striking difference in the behavior of these minimal velocities is the presence of waves propagating with a given speed in the total absence of diffusion ($\Gamma=0$), when only nonlocal reactive dynamics is considered. The numerical integration (Fig. 2) of the discrete equation (13) fully confirms this conclusion. We have here a reaction-induced propagation mechanism to which one may associate a concentration-dependent effective diffusion coefficient subsisting as long as the second-order reaction takes place, even when the hopping probability toward adjacent units is strictly zero. In other words, in such systems, reaction can be seen as being itself a mode of spatial communication. We note that in the continuous limit this effect is penalized by a factor a^2 which was previously supposed to be small. We suggest that Eq. (16) can nevertheless be regarded as a generic equation where a plays the role of a parameter just like k_1 and k_2.

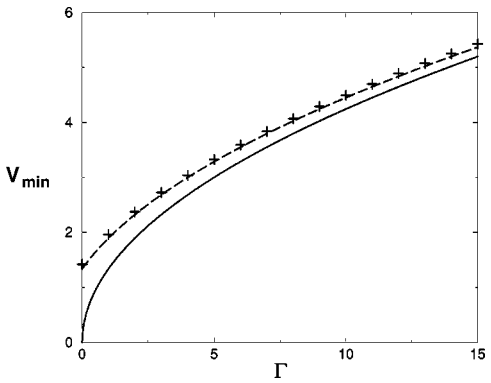

FIG. 2. Evolution of v_{min} as a function of Γ, obtained from the integration of Eq. (12) (dashed line), from the analytical prediction [Eq. (17)] with $a=1$ (crosses), and from classical discrete MA equations (plain line). Parameters k_1, k_2, initial condition, units and system size are as shown in Fig. 1.

IV. WAVE FRONTS BETWEEN TWO STABLE STATES

We consider now a scheme including a third-order step in addition to the bimolecular ones studied in the preceding section,

$$X_2(i) + X_1(i\pm 1) \rightarrow X_1(i) + X_1(i\pm 1) \quad k_1, \tag{19}$$

$$X_1(i) + X_2(i+1) + X_2(i-1) \rightarrow X_2(i) + X_2(i+1) + X_2(i-1) \quad k_2, \tag{20}$$

$$X_1(i) + X_2(i\pm 1) \rightleftharpoons X_2(i) + X_1(i\pm 1) \quad \Gamma, \tag{21}$$

hereafter referred as "trimolecular-bimolecular" model, and where X_1, X_2 can be interpreted in a similar way as before.

A. Formulation and numerical results

Taking into account that $c_1(i)+c_2(i)=1$, the corresponding classical MA rate equation reads in its continuous limit

$$\frac{\partial}{\partial t}\, c = k_1 c(1-c) - k_2 c(1-c)^2 + \frac{\Gamma a^2}{2}\,\nabla^2 c. \tag{22}$$

It displays a cubic local evolution law admitting three homogeneous steady states if $k_2 \geqslant k_1$: $c_1=1$, and $c_3=0$ which are stable, and $c_2=(k_2-k_1)/k_2$ which is unstable. The analysis of the kinetic potential $\mathcal{U}[c]$ shows that c_3 is more stable than c_1 if $k_2>2k_1$, and vice versa. Owing to the cubic form of $f(c)$ there exists a unique propagation velocity of the front between these two stable states in the case of a spatially extended system. If the initial condition is such that

$$c(r,0) = c_1 \quad \text{as} \quad r \rightarrow -\infty, \tag{23}$$

$$c(r,0) = c_3 \quad \text{as} \quad r \rightarrow +\infty, \tag{24}$$

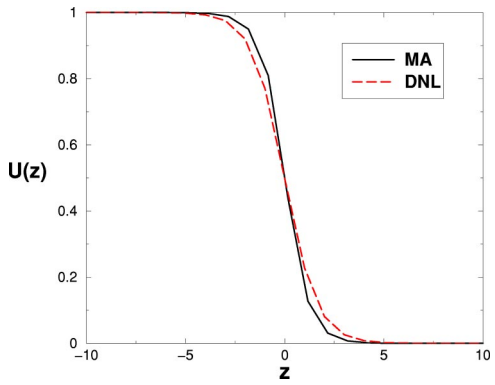

FIG. 3. Shape of the front between the two stable states of the trimolecular-bimolecular model, with $k_1=0.1$, $k_2=0.25$, and $\Gamma=0.1$ (the size is the same as in Figs. 1 and 2). The results are obtained from the discretized version of mass-action rate Eq. (22) (MA) and the discrete nonlocal dynamics [DNL, Eq. (26)]. The initial condition is as in Eqs. (23) and (24), dimensionless units are in force and the network is composed of 10 000 sites.

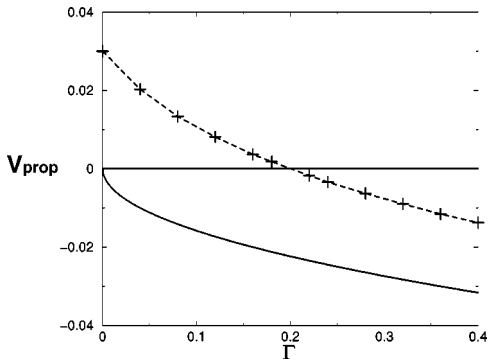

FIG. 4. Propagation velocity as a function of Γ for the TBM model, taken from the MA predictions [Eq. (25)] (full line) and from integration of the DNL equation (26) (dashed line and crosses). The parameters k_1 and $k_2=0.25$, the initial condition, units and the size of the system are identical to those in Fig. 3.

a wave will propagate with velocity

$$v_{\text{prop}}^{\text{MA}}=\sqrt{\frac{k_2\Gamma a^2}{4}}\left(\frac{2k_1-k_2}{k_2}\right). \tag{25}$$

One can check that, if $k_2>2k_1$, $v_{\text{prop}}^{\text{MA}}$ is negative, which means that the more stable state c_3 invades the region with coverage c_1.

The discrete and nonlocal model is on the other hand governed by the evolution equation

$$\frac{d}{dt}c_i=\frac{k_1}{2}(1-c_i)(c_{i+1}+c_{i-1})-k_2c_i(1-c_{i+1})(1-c_{i-1}) + \frac{\Gamma}{2}(c_{i+1}+c_{i-1}-2c_i) \tag{26}$$

whose continuous limit (up to order a^2) reads

$$\frac{\partial}{\partial t}c=k_1c(1-c)-k_2c(1-c)^2+a^2k_2c(\nabla c)^2 + a^2\left[\frac{\Gamma}{2}+\frac{k_1}{2}(1-c)+k_2c(1-c)\right]\nabla^2c. \tag{27}$$

In addition to a density-dependent diffusion coefficient this equation displays a nonlinear ''friction'' term of the form $a^2k_2c(\nabla c)^2$ as expected from Eq. (4). One can easily check that, as anticipated in Sec. II, owing to the nonlinear spatial coupling induced by reaction Eq. (26) does not share the property of the mean-field Eq. (22) to derive from a potential. Furthermore, in absence of mass transfer by diffusion ($\Gamma=0$) it admits a pronounced multiplicity of inhomogeneous steady sates, corresponding to isolated lattice sites occupied by X_1 interrupted by islands of empty sites X_2 comprising at least the first neighbors of the occupied sites.

Figure 3 depicts the result of numerical integration of Eq. (22) (full line) and Eq. (26) on a discrete lattice (dashed line). As can be seen waves with a given front shape and constant velocity are indeed observed. On the other hand, when the full discrete system dynamics is considered, the direction of propagation can be reversed compared to that of the traditional mean-field waves when classical diffusion is weak, as seen in Fig. 4. Specifically, for a given initial condition of the lattice, consider $k_2>2k_1$. The state c_3 should then be the most stable state and invade the region where the concentration is c_1, the velocity of the front being negative. In contrast, we observe that for small hopping probability Γ in the discrete dynamics the *homogeneously less stable state* invades the other one, while the usual behavior is recovered for high diffusion probability. The classical mean-field rate equations are thus inadequate in this case, since they predict exactly the opposite of what is observed in a certain parametric region.

The origin of this discrepancy is to be sought in the system's geometry. With the initial condition chosen (network fully covered on one side and empty on the other side) and in the total absence of diffusion, particles located at the boundary or within the fully covered zone cannot desorb through the trimolecular step. The system behaves as if the first autocatalytic step only were effective (rate k_1). If so, one expects the wave to travel indeed in the observed direction, since $c=1$ is then the only stable state. If this simple explanation holds, one should expect that the wave propagates as predicted by the mean-field if only one full site is initially present in an otherwise empty surface, or if the dynamics takes place on a lattice of higher connectivity allowing for favorable configurations for the trimolecular step. Numerical investigations (not shown here) indicate that it is indeed so, or at least that the direction of propagation is as previously expected.

B. Analytical approach

We may take advantage of the continuous limit in order to gain an analytical understanding of the front propagation. In one space dimension and after eliminating a by redefining the space variable ($r\rightarrow r/a$), Eq. (27) becomes

$$\frac{\partial}{\partial t}c = c(1-c)[k_1 - k_2(1-c)] + k_2 c(\nabla c)^2 + \frac{1}{2}[\Gamma + k_1(1-c) + 2k_2 c(1-c)]\nabla^2 c. \quad (28)$$

We propose to determine an asymptotic approximation of the front solution valid for small values of k_1 and k_2. Specifically, we introduce the small parameter ε and $\kappa = O(1)$ defined by

$$\varepsilon \equiv k_1 \text{ and } \quad k_2 = \varepsilon\kappa, \quad (29)$$

and seek for a traveling wave solution $c = c(z,\varepsilon)$, where z is given by

$$z \equiv \sqrt{\varepsilon} r - v\varepsilon t. \quad (30)$$

In terms of Eqs. (29) and (30), Eq. (28) can be rewritten as

$$-vc' = c(1-c)[1-\kappa(1-c)] + \varepsilon\kappa c c'^2 + \frac{1}{2}[\Gamma + \varepsilon(1-c) + 2\varepsilon\kappa c(1-c)]c'', \quad (31)$$

where prime means differentiation with respect to z. Without loss of generality, we consider the boundary conditions introduced earlier

$$c(-\infty) = 1 \text{ and } \quad c(\infty) = 0. \quad (32)$$

Setting $\varepsilon = 0$ reduces Eq. (31) to the Fisher-Kolmogorov equation with cubic nonlinearity and constant diffusion. The mean-field description is therefore recovered in this limit. If one further sets $v = 0$, Eq. (31) admits the simple front solution joining the two stable states

$$c = c_0(z) = \frac{1}{1 + \exp(\sqrt{2\Gamma^{-1}}z)} \quad (33)$$

provided that

$$\kappa = \kappa_0 = 2. \quad (34)$$

which is the coexistence condition as given by the mean-field approximation. In order to find the effect of κ as it deviates from κ_0 we seek for a solution in the form of a slowly propagating wave, expressed as a perturbative series in ε,

$$c = c_0(z) + \varepsilon c_1(z) + \cdots, \quad v = \varepsilon v_1 + \cdots, \quad \kappa = 2 + \varepsilon\kappa_1 + \cdots. \quad (35)$$

Inserting Eq. (35) into Eq. (31) and equating to zero the coefficients of each power of ε one obtains an equation for c_1 in the form

$$(-1 + 6c_0 - 6c_0^2)c_1 + \frac{1}{2}\Gamma c_1'' = R, \quad (36)$$

where the right-hand side R displays the nonlinear terms generated by discreteness and nonlocality. It is given by

$$R \equiv -v_1 c_0' + \kappa_1 c_0(1-c_0)^2 - 2c_0(c_0')^2 - \frac{1}{2}(1-c_0)(1+4c_0)c_0''. \quad (37)$$

Note that the left-hand side of Eq. (36) admits the nontrivial solution $c_1 = c_0'$. Solvability of Eq. (36) (a bounded solution for $z \to \pm\infty$) then requires the condition

$$\int_{-\infty}^{\infty} R(z) c_0' dz = 0. \quad (38)$$

Using Eqs. (37) and (33) and evaluating the integral in Eq. (38), we obtain an equation for the velocity given by

$$v_1 = -\frac{1}{2}\sqrt{\frac{\Gamma}{2}}(\kappa_1 - \Gamma^{-1}). \quad (39)$$

We note that for large Γ v_1 is negative and proportional to $\sqrt{\Gamma}$. This can be expected from Eq. (28) since the diffusion coefficient is constant in this limit. The new point is however that v_1 may change sign as Γ decreases, in agreement with the numerical findings depicted in Fig. 4. Specifically, v_1 changes sign at $\Gamma = \Gamma_c$ where

$$\Gamma_c = \kappa_1^{-1} \text{and } \quad \kappa_1 > 0. \quad (40)$$

The second condition implies that $k_2 > 2k_1$, a condition that we discussed in the beginning of Sec. IV. The values of the parameters used for the numerical study in Fig. 4 are $k_1 = 0.1$ and $k_2 = 0.25$ meaning, using Eq. (29), $\varepsilon = 0.1$ and $\kappa = 2.5$. From the expansion of κ in Eq. (35), we determine $\kappa_1 = 5$. Then from Eq. (40), we obtain $\Gamma_c = 0.20\ldots$ which is very close to the numerical estimate in Fig. 4 ($\Gamma_c \approx 0.2006$). The nonlinear terms coming from the discrete and nonlocal model all contribute to the Γ^{-1} term in Eq. (39). If $\Gamma \to 0$, $v_1 \to \infty$ and the asymptotic expansion of the solution assuming $v_1 = O(1)$ is no more valid.

We may conclude by noting that the presence of nonlinear propagation terms modify locally the relative stability between the two considered states. This is further illustrated by multiplying both sides of Eq. (6) by $U'(z)$ and subsequently integrating over z from $-\infty$ to $+\infty$. In the usual mean-field limit, the velocity is then given by

$$v_{\text{prop}}^{\text{MA}} = \frac{\mathcal{U}[c_1] - \mathcal{U}[c_3]}{\int_{-\infty}^{+\infty}[U'(z)]^2 dz}$$

and thus the sign of $v_{\text{prop}}^{\text{MA}}$ is directly related to the relative stability given by the difference of the kinetic potentials taken at c_1 and c_3, respectively. On the other hand, when considering the generic evolution law, one obtains

$$v_{\mathrm{prop}}^{\mathrm{CNL}} = \frac{\mathcal{U}[c_1]-\mathcal{U}[c_3]}{\int_{-\infty}^{+\infty}[U'(z)]^2 dz} - \frac{\int_{-\infty}^{+\infty}[g(U(z))[U'(z)]^3 + D(U(z))U''(z)U'(z)]dz}{\int_{-\infty}^{+\infty}[U'(z)]^2 dz}$$

indicating that the direction of propagation of the waves also depends on the nonlocal, nonlinear terms. This could be seen as the intrinsic cause of the discrepancies observed when relying on the predictions made in the mean-field limit.

The stabilization of a metastable state found in our analysis is reminiscent of the noise-enhanced stability of such states recently reported by some authors (Ref. [34] and references therein). One might indeed argue that the spatial degrees of freedom play here the role of an ''effective noise'' coupled to the homogeneous dynamics in a sufficiently intricate (multiplicative) manner to affect stability. On the other hand, there are major differences related to the nonexistence of potential in the present work, contrary to Ref. [34]. Further analysis is necessary to determine whether the two phenomena are merely analogous or, rather, share some quantitative features.

V. CONCLUSIONS

We have investigated the role played by nonlinear and nonlocal reactive dynamics in the propagation of waves on one-dimensional lattices. We have shown that the form of communication induced by such interactions introduces time and space scales which could radically differ from those expected when only diffusive transport is considered. In particular, the examples studied show that the value of the velocity, the shape of the front as well as the direction of propagation itself can differ from the predictions made using the usual reaction-diffusion evolution laws. The analysis of the evolution equations for such systems reveals the presence of process-dependent nonlinear spatial terms, highlighting the role played by nonlocal dynamics as a specific means of spatial communication. The spatially continuous limit of the discrete evolution laws allows for an analytical understanding of the observed deviations: as a rule, the nonlinear spatial terms induce locally a nontrivial modification of the stability of the homogeneous steady states.

Our analysis can be extended in several directions. A comprehensive study of the discretized Eq. (2) and its continuous limit [Eq. (4)] remains to be done. It would also be desirable to clarify their status from the standpoint of thermodynamics and statistical mechanics, including the conditions of existence of a potential functional generating the evolution equations.

From the point of view of the applications our results could provide the basis for the understanding of certain unexpected results obtained in experiments and microscopic simulations of surface processes, like the propagation of waves and the formation of clusters in the case of reactions between immobile adsorbates (Refs. [15–24]). In addition, the modified local stability of the steady states could explain the displacement of bifurcation points from predictions of the mean-field observed in many instances (like, e.g., in Ref. [24]).

Nonlinear diffusion and discreteness are especially relevant in biology. The density dependence of mobility coefficients as they appear in the traditional reaction-diffusion setting of certain problems in population dynamics accounts for a variety of effects, such as crowding and chemotaxis [9]. Beyond this rather classical effect our analysis suggests that the reaction-diffusion equations usually employed in, among others, ecology and epidemics [10–12], population dynamics [27–30], or bacterial growth [31,32] need to be amended when the mobility of the species involved becomes low. Finally, in several problems of interest in biology [5–7], the propagation of information involves chains of immobile units (like cells or neurons) and could thus rely not only on diffusion but also on direct interactions between neighboring entities [33].

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