Tunable Pinning of Burst-Waves in Extended Systems with Discrete Sources

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We study the dynamics of waves in a system of diffusively coupled discrete nonlinear sources. We show that the system exhibits burst waves which are periodic in a traveling-wave reference frame. We demonstrate that the burst waves are pinned if the diffusive coupling is below a critical value. When the coupling crosses the critical value the system undergoes a depinning instability via a saddle-node bifurcation, and the wave begins to move. We obtain the universal scaling for the mean wave velocity just above threshold.

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The effect of discrete source distribution for spatially extended systems is a problem of interest in such disparate fields as the biophysics of the calcium release waves in living cells \[ \delta \] pinning in the dislocation motion in crystals \[ \delta \], breathers in nonlinear crystal lattices \[ \delta \], Josephson junction arrays \[ \delta \], and charge density waves in one-dimensional strongly correlated electron systems \[ \delta \]. In order to elucidate the effects of discreteness, complex models of calcium release have been solved numerically \[ \delta \]. The simple “fire-diffuse-fire” model constructed in \[ \delta \] displays burst (or saltatory) wave fronts. These fronts either propagate or they do not exist: they cannot undergo pinning. If a system with wave pinning consists of diffusively coupled discrete sources \[ \delta \], the standard approach to its analysis has been to completely discretize the dynamics. This is done by replacing the diffusion term with a difference scheme for the field at the source sites \[ \delta \]. This simplification neglects the field structure between sites. The latter is crucial for an understanding of the system dynamics and universal behavior near the pinning/depinning transition.

In this Letter we consider a discrete array of nonlinear reaction sites embedded in a continuum in which the reactant diffuses. We study both analytically and numerically the propagation of burst waves and their pinning, as well as the universal behavior of the system near the pinning threshold. Our model is represented by the following diffusion equation with discrete nonlinear sources (in \( N \)-dimensional space):

\[
 u_t = D \nabla^2 u + \alpha d^N \sum_i \delta(\mathbf{x} - \mathbf{x}_i) f(u),
\]

where \( u \) is a dimensionless concentration, \( D \) is the diffusion coefficient, \( \alpha \) is the production rate of the reactant, and \( d \) is the distance between neighboring sites (channels). These sites are located at \( \mathbf{x}_i \)'s. The reaction dynamics are specified by a nonlinear function \( f(u) \). To describe the waves of one stable phase propagating into another stable phase, we choose the bistable reaction dynamics \[ \delta \]. The simplest example of bistability is given by \( f(u) = -u(u - u_0)(u - 1) \), with two stable fixed points \( u = 0, 1 \), and one unstable fixed point \( u = u_0 \).

In the present Letter we study one-dimensional (1D) wave propagation. Then, after rescaling \( x = \tilde{x}d, t = \tilde{t}\alpha^{-1} \), we obtain from Eq. (1) (after dropping tildes)

\[
 u_t = \beta u_{xx} + \sum_i \delta(x - i) f(u),
\]

with the effective dimensionless diffusion coefficient \( \beta = D/\alpha d^2 \). The system dynamics are determined by the balance between the dissipation and the local nonlinear forcing. The latter can be expressed through its potential as \( f = -dF/du \). The potential \( F(u) \) for a bistable system possesses two minima (stable fixed points of the reaction), separated by a maximum (unstable fixed point of the reaction). For cubic forcing the two minima, \( u = 0, 1 \), have equal energy if the potential is symmetric, i.e. \( u_0 = 1/2 \). In this case no long-time wave propagation is possible. The energy source for the motion is the difference between the depths of the potential minima, as determined by \( \gamma = 1/2 - u_0 \) (for small \( \gamma \) it is \( \sim \gamma \)). For \( \gamma > 0 \), \( u = 0 \) is a local minimum and \( u = 1 \) a global minimum. For \( \gamma < 0 \), the dynamics are analogous but the two minima exchange their roles. We are left, therefore, with two dimensionless parameters which control the behavior of our system: \( \beta \) and \( \gamma \).

In Eq. (2), the effective diffusion coefficient \( \beta \) is the only measure of how close the system is to its continuum limit, \( u_t = \beta u_{xx} + F(u) \), which is realized when \( \beta \to \infty \). The continuous system possesses traveling-wave kink solutions propagating from the locally stable minimum to the globally stable minimum (see, e.g., \[ \delta \]). For small \( \gamma \) this solution has the form \( u = 1/2 [1 - \tanh(z/2\sqrt{\beta})] + O(\gamma) \) (in the traveling wave coordinate \( z = x - Ct \)), and the propagation velocity is \( C \sim \gamma^{1/2} \) \[ \delta \].

Here we investigate the dynamics for all \( \beta \), including the discrete limit, when \( \beta \ll 1 \) for which the dynamics are more complicated. We have performed numerical simulations of Eq. (2). To get rid of the singular form of the dynamics and to ensure convergence with
mesh refinement, we have rewritten the equation in terms of a nonlocal function $U(x, t) = \int_0^L G(x, x') u(x', t) \, dx$, where $L$ is the system length and $G$ is a Green-function of 1D Laplace operator, with no-flux boundary condition $u_x = 0$ at $x = 0$ and Dirichlet boundary condition $u = 0$ at $x = L$. The Green-function has the form $G(x, x') = (x - x') H(x - x') + x' - L$ with $H$ being a step-function. Equation for $U(x, t)$ was integrated implicitly, and the inverse Green-function used to restore $u(x, t)$ needed to calculate the nonlinearity.

Far from the continuum limit the system exhibits well developed burst waves. Figure 1 shows a space-time plot of the solution $u(x, t)$ in the burst-wave regime. These burst waves are propagating solutions which, in the appropriate co-moving reference frame, are strictly periodic. The bursting period is uniquely determined by $\beta$ and $\gamma$.

![Space-time plot of u(x, t)](image)

**FIG. 1.** Space-time plot of $u(x, t)$, with black corresponding to $u = 1$ and white to $u = 0$. Time goes positive downward. Parameters of our model are $\beta = 0.017$, $\gamma = 0.3$ ($u_0 = 0.2$). The system length is $L = 20$, and number of the grid-points is 1000. Time step $dt \approx 0.007$. The period of the bursting is $T = 35.28$, total simulation time is $3T$.

For small enough $\beta$ the burst waves are pinned. A pinned solution of Eq. (2) is a static piece-wise linear curve connecting the stable states $u = 1$ and $u = 0$. The solution of the 1D Laplace equation is linear, so the sites are the points where the second derivative is proportional to the $\delta$-function. Thus the problem is reduced to a set of algebraic equations on the values of $u$ at the sites

$$\beta (u_{i+1} + u_{i-1} - 2u_i) + f(u_i) = 0,$$

where $u_i = u(x_i)$.

We define the first site (going from $u = 1$ to $u = 0$) where the second derivative of $u$ is positive as “the front”, with corresponding site number $m$. In the discrete limit ($\beta \ll 1$) it can be shown that the values of $u$ at the sites approach 1 (0) exponentially with distance from the front. In particular, $u_{m+i} \sim \beta^i$ and $1 - u_{m-i} \sim \beta^i$. Let us consider the problem of pinning to first order in $\beta$. Then Eq. (3) at the front becomes $g = u_m u_m (u_0 + 1) + u_0 + 2\beta - \beta = O(\beta^2)$. In Figure 2 we plot $g(u_m)$. By definition of $u_m$, $(u_m)_{xx} > 0$, thus it follows from Eq. (3) that $u_m < u_0$. Therefore, the rightmost root is not appropriate and the existence of solution depends on the value of $\beta$. The critical value of $\beta$, $\beta_c$, at which stationary solutions cease to exist, corresponds to the situation when two remaining roots of $g(u_m)$, $u_m = u^-$ and $u_m = u^+$ merge at the graph maximum $u = u_{max}$.

![Graphical representation of g(u_m)](image)

**FIG. 2.** A graphical representation of $g(u_m)$ used to solve the stationary problem (1) to the first order in $\beta$. Parameter $\gamma = 0.1$ ($u_0 = 0.4$). Stable (unstable) front solution corresponds to $u_m = u^-$ ($u^+$).

The stability of a stationary solution of Eq. (2), $u^*_i$ ($i = 1, 2, \ldots$), is determined by the eigenvalues of the system obtained by linearizing system (3). This yields the maximum eigenvalue $\lambda_{max} = f_u(u_m) - 2\beta + O(\beta^2)$ which, for the roots $u_m = u^-$ and $u_m = u^+$, is negative and positive, respectively. Since all remaining eigenvalues are negative, $u = u^+$ is a saddle and $u = u^-$ is a node (see Fig. 3). If we substitute $\beta = \beta_c$ in the expression for $\lambda_{max}$ we find that $\lambda_{max} = 0$ (see the definition of $g(u_m)$). That is, the stability boundary for the stationary solution coincides with that of its existence. This implies that the pinning/depinning instability occurs via saddle-node bifurcation.

An analysis similar to the above, but to second order in $\beta$, yields the bifurcation line for the pinning/depinning transition in $(\gamma, \beta)$ space. In Figure 3 we compare the analytical bifurcation line with that obtained by direct numerical simulations of Eq. (2). As shown in the figure, the theory is in good quantitative agreement with the simulations, even beyond the applicability of the small $\beta$ perturbation theory developed above. For $\gamma \to 0$, the
energy source of wave motion vanishes and consequently $\beta_c$ diverges.

Let us now study the universal behavior of our system near the critical diffusion coefficient $\beta = \beta_c$. First we note that the system dynamics are variational, i.e.,

$$\frac{\partial u}{\partial t} = -\frac{\delta E[u]}{\delta u},$$

where $\delta / \delta u$ is a variational derivative in the space of functions $u(x)$ of a nonlinear functional $E[u]$, given by

$$E[u] = \frac{\beta}{2} \int (\frac{\partial u}{\partial x})^2 dx + \sum_i F[u(i)].$$

This functional diverges for infinite systems. Therefore we use only its difference for different functions $u(x)$.

Denote a small deviation of $\beta$ from the critical value as $\epsilon = \beta - \beta_c$ and consider first the case of $\epsilon < 0$. Then, diffusion is not strong enough to cause wave propagation, and there exists a linearly stable stationary kink solution $u_s(x)$, corresponding to $u^-$ in Figure 3. Let $u^n(x)$ be a function obtained by translating $u(x)$, such that $u^n(x) = u(x+n)$. If $u_s(x)$ is a minimum of $E[u]$ then $u^n_s(x)$ is also a minimum of $E[u]$ for any integer $n$, implying that the functional $E[u]$ has an infinite set of minima. One can show that $E[u^n_s(x)] - E[u_s(x)] = F(u \equiv 1) - F(u \equiv 0)$.

Consider two adjacent minima of $E[u]$, $u_s(x)$ and $u^1_s(x)$. The corresponding basins of attractions have a common boundary. A minimum of $E[u]$ on the boundary is a saddle point $u_0(x)$ of the functional $E[u]$, which represents an unstable kink, corresponding to $u^+$ in Figure 3. Due to the discrete translational symmetry of the system, $u^n_0(x)$ is also a saddle point of $E[u]$ for any integer $n$. A variation of the functional $E[u]$ in a vicinity of the unstable kink $u_n(x)$ is represented by a quadratic form (in the variation of the function), having one negative eigenvalue and a corresponding unstable direction $\mathbf{n}$. There exist two separatrix lines of $E[u]$, $L_1$ and $L_2$, which start at $u_n$ and go to $u_s$ and $u^1_s$, respectively. The tangent directions of the separatrices at $u_n$ are collinear to $\mathbf{n}$. The curve $L_{12} = L_1 \cup L_2$ joins two stable minima $u_s$ and $u^1_s$, and contains the saddle $u_n$. If we continue this curve infinitely it will contain all nodes and saddles of $E[u]$.

Let us introduce a normal coordinate (arc-length) $s$ on this curve, $ds^2 = dt^2 \int (\partial u / \partial t)^2 dx$. Figure 4(a) shows $E(s)$ obtained numerically for $\epsilon < 0$. The minima and maxima of $E(s)$ [see inset in Fig. 4(a)] correspond to stable kinks $u_s$ and unstable kinks $u_n$, respectively. It can be shown, using the definitions of $E$ and $s$, that the system dynamics on the trajectory is governed by

$$\frac{ds}{dt} = -\frac{dE}{ds}.$$
where $s_0$ is a finite constant.

For small $\epsilon$, $T$ in (6) does not depend on $s_0$ and is $\sim 1/\sqrt{\epsilon}$. Therefore, the average kink velocity is $C = 1/T \sim \sqrt{\epsilon}$ near the bifurcation point. Fig. 3 is a plot of the velocity $C$ as a function of $\epsilon = \beta - \beta_c$ obtained by numerical simulations of Eq. (5). The $\sqrt{\epsilon}$-scaling near the critical point is clearly seen. For finite $\epsilon$, the scaling breaks and, after a transient range of $\beta$, the expected continuum scaling $C \sim \sqrt{\beta}$ appears.

If we identify the set of points $x + n$ as one point, a moving kink will be a periodic trajectory (limit cycle) on the reduced manifold, born by a saddle-node bifurcation. This type of behavior is well known for finite-dimensional systems [10]. A simple exactly soluble example which has both the symmetries and the scaling behavior discussed here is given by $dx/dt = 1 + (1 - \epsilon) \cos 2\pi x$. For $\epsilon < 0$ the system has an infinity of fixed points and for $\epsilon > 0$ the fixed points cease to exist and the solution propagates with $x(t + T) = x(t) + 1$ and $T \sim 1/\sqrt{\epsilon}$ for small $\epsilon$.

![FIG. 5. Wave propagation velocity $C$ vs $\beta - \beta_c$ (solid line). Dashed lines with slope 1/2 show the scalings $C \sim \sqrt{\epsilon} = \sqrt{\beta - \beta_c}$ and $C \sim \sqrt{\beta}$ for discrete and continuous domain, respectively. Dashed-dotted lines illustrate the boundaries of continuous, discrete, and transient domains of $\beta$. The parameters are $\gamma = 0.1$ and $\beta_c \approx 0.0617$.](http://www-xde.lanl.gov/XCM/pearson/dfd.html)

We have shown that there exist standing kink solutions for one-component bistable reaction-diffusion systems with discrete sources. We have also obtained the universal scaling for the mean velocity just above the pinning threshold. We conjecture that pinning is universal in all bistable systems with discrete sources. Pinning was also observed in numerical simulations of a nonvariational but bistable model for the calcium release wave in cardiac myocytes [11]. These results are in contrast to those in [10] and [12] in which saltatory or burst waves were found with the velocity scaling as $C \sim D/d$ for small $\beta$, but no pinning. The systems in [10] and [12] were not bistable which is consistent with our conjecture. In all models studied so far, waves fail to propagate for large enough site spacing. The manner in which propagation failure occurs differs from system to system. For example in the “fire-diffuse-fire” model [12] of calcium dynamics, propagation failure occurs through a sequence of period-doubling bifurcations and crises. These facts raise an interesting open question. In what ways can waves fail to propagate as the source spacing is increased? To this end it would be useful to systematically generalize the work here to nonvariational systems. Such systems would be also more realistic as models of calcium dynamics in living cells.

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[1] N. Callamaras, J. S. Marchant, X.-P. Sun, and I. Parker, J. Physiol. 509, 81 (1998); R. B. Silver, Cell Calcium 20(2), 161 (1996).
[2] G. Dupont and A. Goldbeter, Biophys. J. 67, 2191 (1992); M. S. Jafri and J. Keizer, Biophys. J. 69, 2139 (1995).
[3] S. Flach and K. Kladko, Phys. Rev. E 54, 2912 (1996).
[4] S. Flach and C. R. Willis, Phys. Rep. 295, 181 (1998).
[5] L. M. Floria and J. J. Mazo, Adv. Phys. 45, 505 (1996).
[6] H. Fukuyama and P. A. Lee, Phys. Rev. B 17, 535 (1978).
[7] S. N. Coppersmith, Phys. Rev. Lett. 65, 1044 (1990).
[8] R. A. Bishop, B. Horovitz, and P. S. Lomdahl, Phys. Rev. B 38, 4853 (1988).
[9] A. E. Bugrim, A. M. Zhabotinsky, and I. R. Epstein, Biophys. J. 73, 2897 (1997).
[10] J. Keizer, G. D. Smith, S. Ponce Dawson, and J. E. Pearson, Biophys. J. 75, 595 (1998); G. D. Smith, thesis, University of California Davis (1996).
[11] P. A. Spino and H. G. Othmer, Bull. Math. Biol. (submitted).
[12] S. Ponce Dawson, J. Keizer, and J. E. Pearson, Proc. Nat. Acad. Sci. (submitted); J. E. Pearson and S. Ponce Dawson, to appear Physica A. http://www-
[13] M. Cross and P. C. Hohenberg, Rev. Mod. Phys. 65 (1993).
[14] A. S. Mikhailov, Foundations of Synergetics I. Distributed Active Systems (Springer-Verlag, Berlin, 1990).
[15] J. J. Tyson and J. P. Keener, Physica D 32, 327 (1988); D. A. Kessler, H. Levine, and W. N. Reynolds, Physica D 70, 115 (1994).
[16] V. I. Arnol’d (Ed.), Dynamical Systems V, Bifurcation Theory (Springer-Verlag, 1994).