KINKS IN A STOCHASTIC PDE

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Abstract We consider a stochastic PDE with localized coherent structures known as kinks. The availability of exact results for the steady state and increasing computer power means that precise quantitative comparison between theory and numerics is possible. One of the quantities of interest is the steady-state density of kinks, maintained by a balance between nucleation and annihilation of kink-antikink pairs. The density as measured from numerical solutions is sufficiently accurate to resolve the difference between analytical predictions based on the exact value of the correlation length, and those based on the WKB approximation to it.

Keywords: Stochastic PDEs, kinks, convergence of algorithms.

Many extended systems have localized coherent structures that maintain their identity as they move about and are buffeted by local fluctuations [1, 2]. To study the dynamics, we must accurately solve nonlinear extended systems with noise and devise a sensible method for identifying and tracking the coherent structures. Until fairly recently, computer memory and performance restrictions were sufficiently severe that stochastic partial differential equations (stochastic PDEs) describing extended systems with noise could only be studied at low resolution. These restrictions are being overcome, at least in one space dimension [3, 4, 5], and good progress has been made towards studying, understanding, and improving the accuracy of numerical solutions.

Numerical solutions of stochastic PDEs are cannot be performed in the infinite-dimensional space in which the equation is defined [6, 7], but

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are carried out in a finite- (but large-) dimensional space obtained by discretizing the spatial coordinate [5]. The set of coupled stochastic differential equations (SDEs) thus obtained is evolved using a timestepping method that discretizes time. Thus a systematic study of the numerics of stochastic partial differential equations requires a study of convergence in both space and time.

In addition to questions of convergence of the numerical scheme, one is often interested in the limit of low noise intensity. This limit is convenient for analytical approximations and for unambiguous identification of coherent structures, but requires large amounts of computer time. Two reasons for the increase in computer time with decreasing temperature are as follows. Firstly, the timescales of the system typically increase exponentially as temperature decreases, so one must perform runs of increasing duration to attain the steady state from an arbitrary initial condition. Secondly, the density of coherent structures also decreases with decreasing temperature, so ever larger systems are needed to obtain good statistics.

In this paper we examine a stochastic PDE in one space dimension that can be written as follows:

$$\frac{\partial}{\partial t}\boldsymbol{\phi}_t(x) - \frac{\partial^2}{\partial x^2}\boldsymbol{\phi}_t(x) = \boldsymbol{\phi}_t(x) - \boldsymbol{\phi}_t^3(x) + (2kT)^{\frac{1}{2}}\,\boldsymbol{\xi}_t(x). \tag{1}$$

The last term in (1) is space-time white noise:

$$\left\langle \boldsymbol{\xi}_t(x)\boldsymbol{\xi}_{t'}(x')\right\rangle = \delta(x-x')\delta(t-t'). \tag{2}$$

Angled brackets indicate mean over realizations. The amplitude of the noise is $(2kT)^{\frac{1}{2}}$ where T has the interpretation of temperature and k is Boltzmann's constant. We shall use the notation $\beta = (kT)^{-1}$. The configuration at time t is a continuous function of x denoted $\boldsymbol{\phi}_t$. The value at time t and position x is a random variable denoted $\boldsymbol{\phi}_t(x)$. Periodic boundary conditions are used in x.

The SPDE (1), known as the ϕ^4 equation with noise, has been extensively studied as a model with nonlinear coherent structures; here we restrict ourselves to one space dimension, where they are known as kinks [2]. The one-dimensional equation, as well as serving as a general model for a chain of coupled double-well oscillators [13], has been used to model specific physical systems such as the polymer polyacetalene [14], charge-density-wave condensates [15], and Josephson-junction transmission lines [16].

In order to solve the SPDE numerically, we first discretize in space, producing a set of coupled SDEs. We use the following notation for the

SDE governing the time evolution of the stochastic process at position x [5]:

$$\mathrm{d}\boldsymbol{\phi}_t(x) = \Big(\boldsymbol{\phi}_t(x) - \boldsymbol{\phi}_t^3(x) + \tilde{\Delta}\boldsymbol{\phi}_t(x)\Big)\,\mathrm{d}t + (2kT)^{\frac{1}{2}}\mathrm{d}\mathbf{B}_t(x), \qquad (3)$$

where $\langle \mathrm{d}\mathbf{B}_t(x)\mathrm{d}\mathbf{B}_{t'}(x')\rangle = \delta(x-x')\delta(t-t')\mathrm{d}t$. The discretized spatial operator is

$$\tilde{\Delta}\boldsymbol{\phi}_t(x) = \big(\boldsymbol{\phi}_t(x+\Delta x) + \boldsymbol{\phi}_t(x-\Delta x) - 2\boldsymbol{\phi}_t(x)\big)\Delta x^{-2},$$

where Δx is separation between neighboring sites. The dynamics of the system discretized in space can be thought of as that of a string of coupled overdamped oscillators subject to three competing influences: a double-well on-site potential, coupling to neighboring sites and random fluctuations.

In order to solve the system discretized in space we also discretize in time and generate a realization of the stochastic PDE, consisting of a long series of discretized configurations. Each discretized configuration consists of $\Phi(t,x)$ at a large number (typically 10^6) of values of x. In the stochastic Runge-Kutta algorithm [8, 9] used for the numerical results in this paper, each site is updated using the following set of temporary values:

$$\begin{aligned}\Psi(t,x) &= \Phi(t,x) + \Big(\Phi(t,x) - \Phi^3(t,x) + \tilde{\Delta}\Phi(t,x)\Big)\,\Delta t \\ &\quad + (2kT)^{\frac{1}{2}}(\Delta t/\Delta x)^{\frac{1}{2}} n(t,x), \end{aligned} \qquad (4)$$

where $n(t,x)$ is drawn from a probability distribution, independently at each x and t. Using the temporary values (4), the update is

$$\begin{aligned}\Phi(t+\Delta t,x) &= \Phi(t,x) + \frac{1}{2}\Big(\Phi(t,x) - \Phi^3(t,x) + \tilde{\Delta}\Phi(t,x)\Big)\,\Delta t \\ &\quad + \frac{1}{2}\Big(\Psi(t,x) - \Psi^3(t,x) + \tilde{\Delta}\Psi(t,x)\Big)\,\Delta t \\ &\quad + (2kT)^{\frac{1}{2}}(\Delta t/\Delta x)^{\frac{1}{2}} n(t,x). \end{aligned} \qquad (5)$$

The distribution of each $n(t,x)$ is either a Gaussian with zero mean and unit variance, or the following three-point distribution:

$$n(t,x) = \begin{cases} -\sqrt{3} & \text{with probability } 1/6 \\ 0 & \text{with probability } 2/3 \\ \sqrt{3} & \text{with probability } 1/6. \end{cases} \qquad (6)$$

Numerical runs with the $n(t,x)$ distributed according to (6) produce results that are indistinguishable, on the scale of Figure 1, from those obtained when the $n(t,x)$ are drawn from a Gaussian distribution.

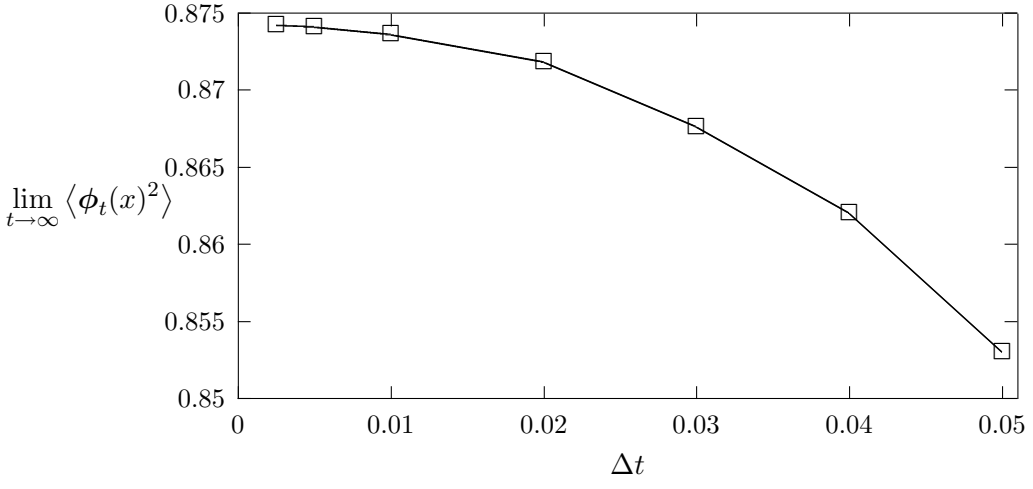

Figure 1. The measured value of $\lim_{t\to\infty} \langle \phi_t^2(x) \rangle$ versus Δt for $\Delta x = 0.4$ and $\beta = 7$.

In numerical realizations of the stochastic evolution described by (3), one finds that the quantity $\langle \phi_t^2(x) \rangle$, the mean square value of the field at an arbitrarily chosen point, attains a well-defined mean value after a relaxation time of order 1 [4]. This value depends both on Δx and on Δt [4]. In Figure 1 we show the dependence of $\lim_{t\to\infty} \langle \phi_t^2(x) \rangle$ on Δt when Δx is fixed.

An example of a part of a configuration (values of $\phi_t(x)$ at one time and a range of values of x) is shown in Figure 2. The configuration consists of long regions where the field is close either to 1 or to -1, occasionally interrupted by narrow interpolating regions. The latter are called kinks if they have a region where the field is negative to the left and one where the field is positive to the right; they are called antikinks if they have a region where the field is positive to the left and one where the field is negative to the right.

Once good accuracy in space and time has been achieved, one turns to the question of identification and counting of kinks. Simply counting zero crossings of the field results in an overestimate of the number of kinks, because kinks and antikinks do not have smooth profiles, and because "phonon" fluctuations in the regions where $\phi_t(x)$ is close to ± 1 are occasionally enough to produce a zero crossing that we would not normally consider to be a kink-antikink pair. In Figure 3, we illustrate one way of dealing with this. At a chosen time in the evolution, a copy of the current configuration is sent to a subroutine that evolves the system,

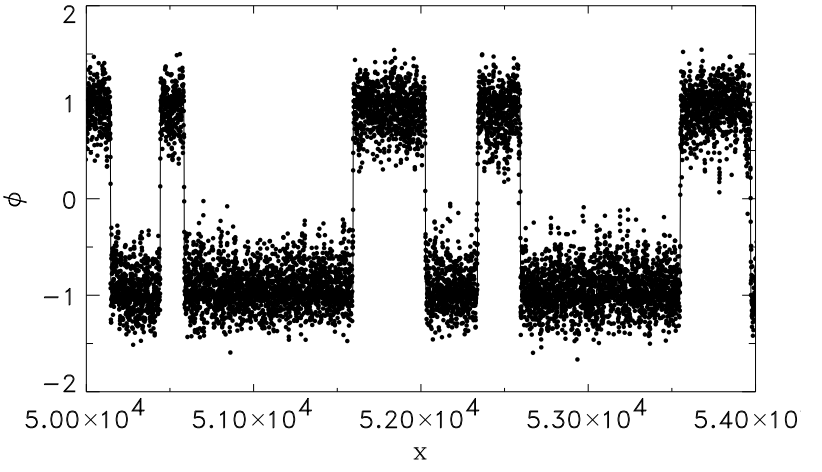

Figure 2. Part of a numerical configuration. The dots are values at grid points. Kinks and antikinks alternate along the x direction. Here $\beta = 8$.

according to (1) but without noise ($T = 0$). The result is a very fast damping of the phonon fluctuations and smoothing of kink profiles that allows the number of kinks to be determined by counting zero crossings. Of course, if this noiseless "cooling" is continued indefinitely, genuine kinks and antikinks will collide and annihilate and the density of kinks will be underestimated. In practice, the separation of timescales is such that it is possible to choose a suitable intermediate value for the cooling time, as long as the equation is being solved at a temperature low enough that kinks are unambiguously defined.

After a relaxation time proportional to $\exp(2E_k\beta)$, where $E_k = (8/9)^{\frac{1}{2}}$, a well-defined steady-state density of kinks (and equal density of antikinks) ρ is established [10, 11, 12]. This mean is dynamically maintained: kinks and antikinks are nucleated in pairs, follow Brownian paths and annihilate on meeting [12, 17, 18]. Under the assumption that kink-antikink pairs are nucleated at random times and positions at rate Γ with separation b, have diffusivity D and annihilate on collision, the mean density as a function of time can be calculated exactly [19]. As $b\rho \to 0$, the steady-state density of kinks is given by

$$\rho = \frac{1}{2}\left(\frac{b\Gamma}{2D}\right)^{\frac{1}{2}}. \tag{7}$$

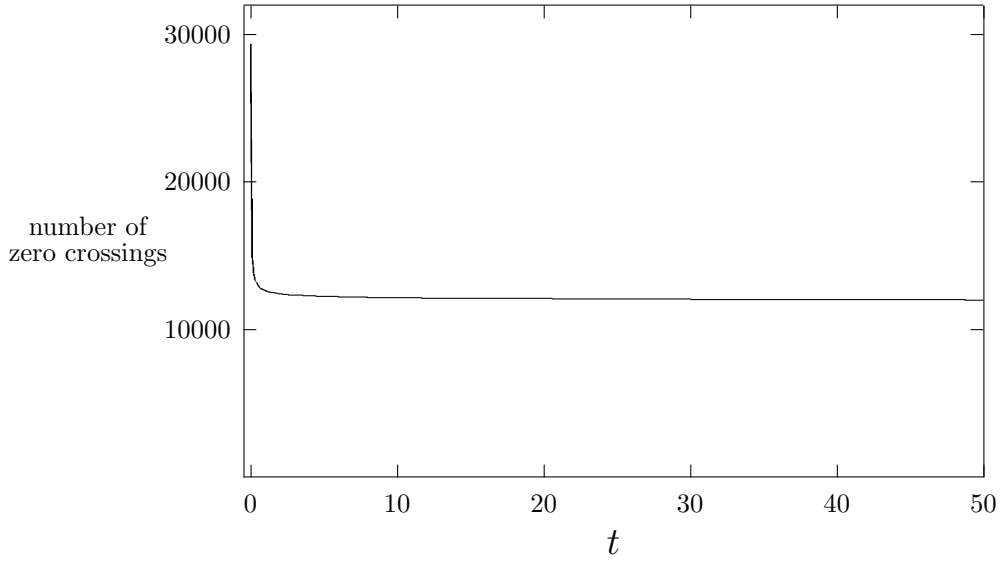

Figure 3. Counting kinks using cooling. The number of zero crossings is plotted as a function of cooling time. The initial rapid decrease corresponds to the damping out of small-scale fluctuations, leaving only the kinks and antikinks. The graph comes from a numerical solution at $\beta = 7$ on a spatial domain with length $L = 2097152$.

At late times the system evolving according to (1) can be thought of as sampling from a steady-state distribution of configurations, calculated as the stationary solution of a Fokker-Planck equation [10, 4]. Consequently, many late-time properties of the solutions of the stochastic PDE can be calculated analytically. For example the correlation function defined by

$$c(x) = \lim_{t\to\infty} \langle \boldsymbol{\phi}_t(y)\boldsymbol{\phi}_t(y+x)\rangle \tag{8}$$

is independent of y. As $x \to \infty$,

$$c(x) \to \exp(-x/\lambda). \tag{9}$$

The correlation length λ is given by

$$\lambda = \left(\beta(\epsilon_1 - \epsilon_0)\right)^{-1}, \tag{10}$$

where ϵ_0 and ϵ_1 are the two smallest eigenvalues of the equation

$$\left(-\frac{1}{2\beta^2}\frac{\partial^2}{\partial u^2} - \frac{1}{2}u^2 + \frac{1}{4}u^4\right)\psi_n(u) = \epsilon_n\psi_n(u). \tag{11}$$

The same method can be used to calculate the dependence of the correlation function on the grid spacing Δx. The lowest order corrections to the continuum in one space dimension are proportional to Δx^2 and equivalent to a corrected on-site potential [20, 4]. An algorithm has been devised, with the potential augmented by a term proportional to Δx^2, that gives improved convergence to the continuum [4, 5].

At sufficiently low temperatures, the lengthscale defined by the inverse density of kinks is very much larger than the typical separation of a kink-antikink pair at the instant of nucleation [17, 12] and the late-time distribution of kinks and antikinks is very close to a random distribution [12, 19]. In such a case, the density of kinks is related to the correlation length λ by

$$\rho = \frac{1}{4}\frac{1}{\lambda}. \tag{12}$$

In Figure 4, we compare the density of kinks as measured from very large numerical solutions with the prediction (12), where λ is given by (10). In the solid line, the eigenvalues ϵ_0 and ϵ_1 are obtained from numerical solution of (11). The dotted line uses the WKB approximation [10] to those eigenvalues. The density as measured from numerical solutions of the stochastic PDE is sufficiently accurate to resolve the difference between the exact value of λ and the WKB approximation to it. The accuracy of the latter approximation improves as the temperature T is lowered. As $T \to 0$, the number of kinks per unit length is proportional to $\exp(-E_k\beta)$.

Performing precise quantitative studies of numerical convergence of thermodynamic properties, where exact analytical results are available, makes it possible to proceed with confidence to an exploration of the fascinating dynamics of individual kinks, where few analytical results are available. Following the spacetime trajectories of individual kinks and antikinks as they are nucleated, diffuse and annihilate on collision, one finds that the mean lifetime of a kink is proportional to $\exp(E_k\beta)$. In order to understand the distribution of lifetimes, it is illuminating to classify each kink's time line according to whether it ends in annihilation with the antikink it was nucleated with, or with some other antikink. The former event is much more likely: the distance between newly nucleated pairs is much smaller than the inverse of the steady-state density of kinks, so their Brownian paths are more likely to intersect [17, 12].

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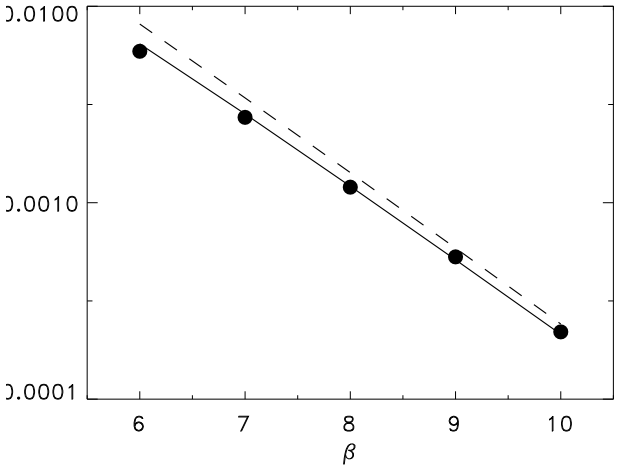

Figure 4. Density of kinks vs inverse temperature (log scale). The dots are densities measured from numerical solutions of the stochastic PDE (1). The solid line is the prediction (12), where the exact correlation length λ is obtained from (10). The dotted line uses the WKB approximation to the eigenvalues of (11).

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