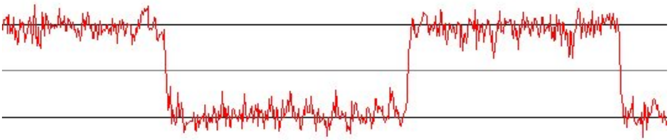
# Kinks and nucleation in a stochastic PDE

Thank you for inviting me!

Grant Lythe

Applied Mathematics, University of Leeds
`http://maths.leeds.ac.uk/~grant`



# Contents



## coauthors


Salman Habib, Los Alamos    Mario Castro, UP Comillas Madrid
Franz Mertens, U Bayreuth    Luis Bettencourt, Los Alamos
Katja Lindenberg, UC San Diego    Carmen Molina-París, Leeds

# Equations of motion

## The $\phi^4$ stochastic PDE can be written

$$\mathrm{d}\mathbf{\Phi}_t(x) = \left(\mathbf{\Phi}_t(x) - \mathbf{\Phi}_t(x)^3 + \partial^2_{xx}\mathbf{\Phi}_t(x)\right)\mathrm{d}t + (2KT)^{\frac{1}{2}}\mathrm{d}\mathbf{W}_t(x),$$

where $x \in [0, L]$ periodic

and $\mathbb{E}(\mathrm{d}\mathbf{W}_t(x)\mathrm{d}\mathbf{W}_{t'}(x')) = \delta(x - x')\delta(t - t')\mathrm{d}t.$

## Discretised using finite differences, it is a system of $N$ SDEs

$$\begin{array}{cccccc} & \leftarrow \Delta x \rightarrow & & & & \\ \ldots\times & \times & \times & \times\ \ldots & & \times \\ & i-1 & i & i+1 & & N \end{array}$$

$$\mathrm{d}\mathbf{\Phi}_t(i) = \Big(\mathbf{\Phi}_t(i) - \mathbf{\Phi}_t(i)^3 + \mathcal{L}_i\mathbf{\Phi}_t\Big)\mathrm{d}t + (2KT/\Delta x)^{\frac{1}{2}}\mathrm{d}\mathbf{W}_t(i),$$

$\mathcal{L}_i\mathbf{\Phi}_t = \Delta x^{-2}(\mathbf{\Phi}_t(i+1) + \mathbf{\Phi}_t(i-1) - 2\mathbf{\Phi}_t(i)),$

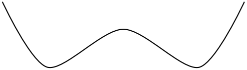
$\mathbb{E}(\mathrm{d}\mathbf{W}_t(i)\mathrm{d}\mathbf{W}_t(i')) = \delta_{i-i'}\,\mathrm{d}t.$ $L = N\Delta x$, and $\beta = 1/KT.$

# Double-well potential and energy

The SPDE can be written

$$\mathrm{d}\boldsymbol{\Phi}_t(x) = \left(-V'(\boldsymbol{\Phi}_t(x)) + \partial_{xx}^2 \boldsymbol{\Phi}_t(x)\right)\mathrm{d}t + \sqrt{2KT}\mathrm{d}\mathbf{W}_t(x),$$

where $V(\phi) = -\frac{1}{2}\phi^2 + \frac{1}{4}\phi^4$,



or

$$\mathrm{d}\boldsymbol{\Phi}_t(x) = -\frac{\delta\mathcal{E}[\boldsymbol{\Phi}_t]}{\delta\boldsymbol{\Phi}_t}\mathrm{d}t + \sqrt{2KT}\mathrm{d}\mathbf{W}_t(x),$$

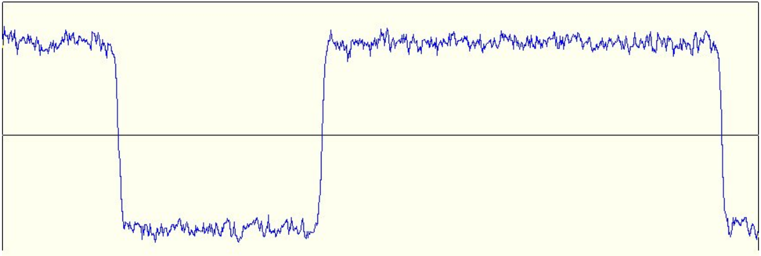
where

$$\mathcal{E}[f] = \int \left(V(f(x)) + \frac{1}{2}\left(\partial_x f(x)\right)^2\right)\mathrm{d}x.$$


Faris and Jona-Lasinio *Large fluctuations for a nonlinear heat equation with noise*
Journal of Physics A (1982)

# kinks and antikinks

…are localised structures interpolating between minima of $V$.



A (noiseless) kink at $x = x_0$,
$\phi^{\mathrm{k}}(x) = \tanh(\frac{x-x_0}{\sqrt{2}})$,
has energy $E_k = \mathcal{E}[\phi^{\mathrm{k}}(x)] = \sqrt{8/9}$.

An antikink at $x = x_0$,
$\phi^{\mathrm{a}}(x) = -\tanh(\frac{x-x_0}{\sqrt{2}})$,
has the same energy.

# The stationary density

The discretized SPDE is a system of $N$ SDEs with a stationary density:

$$r(\phi(1),\ldots,\phi(N)) = Z^{-1}\exp\left(-\beta H(\phi(1),\ldots,\phi(N))\right),$$

where

$$H(\phi(1),\ldots,\phi(N)) = \sum_{i=0}^{N}\left(\frac{1}{2}\frac{(\phi(i+1)-\phi(i))^2}{\Delta x^2} - \frac{1}{2}\phi^2(i) + \frac{1}{4}\phi^4(i)\right).$$

The normalization constant to be calculated is

$$Z = \int_{-\infty}^{\infty}\ldots\int_{-\infty}^{\infty}\prod_{i=1}^{N} T(\phi(i),\phi(i+1))\,\mathrm{d}\phi(1)\ldots\mathrm{d}\phi(N),$$

where

$$T(\phi,\phi') = \exp\left(-\tfrac{1}{2}\beta\Delta x\left(\left(\frac{\phi'-\phi}{\Delta x}\right)^2 + V(\phi) + V(\phi')\right)\right).$$

# The transfer integral method

Calculation of $Z$ is reduced to an eigenvalue problem.
If we can find the $\psi_n$ and $t_n$ such that

$$\int_{-\infty}^{\infty} T(\phi, \phi')\psi_n(\phi)\mathrm{d}\phi = t_n\psi_n(\phi'),$$

we can write $T(\phi, \phi') = \sum_n t_n\psi_n(\phi)\psi_n(\phi')$ and $Z = \sum_n t_n^N$.

Suppose $t_0 > t_1 \ldots > t_N$. Then, as $N \to \infty$, $Z \simeq t_0^N$.

## Auxiliary Schrodinger equation

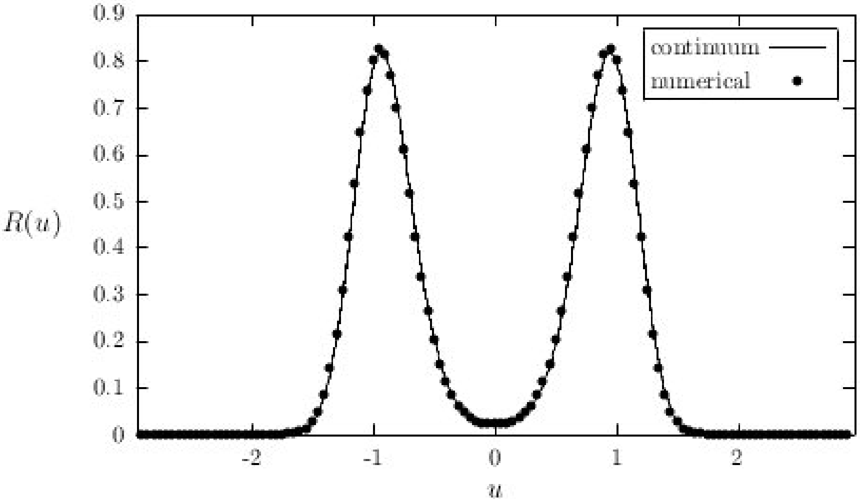
Let $t_n = \mathrm{e}^{-\beta \Delta x \epsilon_n}$. As $\Delta x \to 0$, the $\epsilon_n$ and $\psi_n$ satisfy

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

As $N \to \infty$, $Z \simeq \mathrm{e}^{-\beta L \epsilon_0}$.

Scalapino, Sears and Ferrell *Statistical Mechanics of One-D Ginzburg-Landau Fields*
Physical Review B **6**, 3409 (1972)

# One-point density

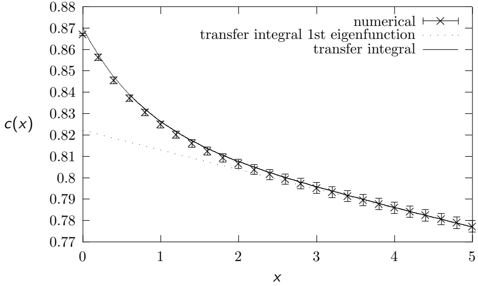


# Correlation function

The correlation function: $c(x) = \lim_{t\to\infty} \mathbb{E}(\mathbf{\Phi}_t(x)\mathbf{\Phi}_t(0))$.

$$c(x) = \sum_n s_n \exp(-\beta|x|(\epsilon_n - \epsilon_0)) \quad \text{where} \quad s_n = \int u\psi_n(u)\psi_0(u)\mathrm{d}u.$$

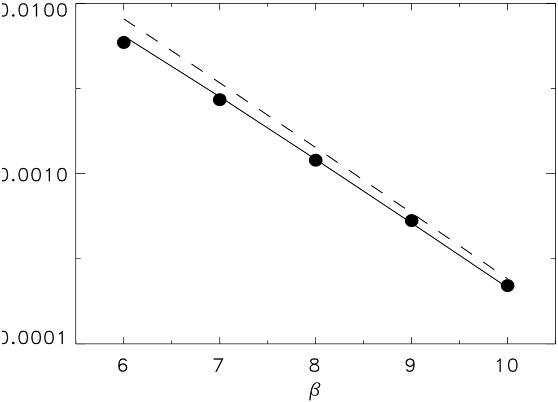
As $x \to \infty$, $c(x) \to s_1 \exp(-x/\lambda)$, where $\lambda^{-1} = \beta(\epsilon_1 - \epsilon_0)$.




Correlation function for $\beta = 7$.


Currie, Krumhansl, Bishop and Trullinger Physical Review B **6 22**, 477 (1980).

# Number of kinks per unit length




(a)

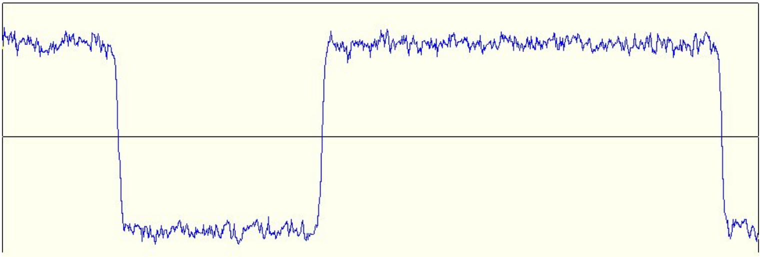
Figure: (a) Kink density vs $\beta$. The dots are obtained from large-scale numerical solutions of the stochastic PDE. The solid line is $\frac{1}{4\lambda}$, where the correlation length $\lambda$ is obtained from the transfer integral. The dashed line is the approximation $\rho \simeq \sqrt{E_k \beta}\exp(-E_k \beta)$.

1. Kinks in the $\phi^4$ SPDE
   - stationary density
   - transfer integral

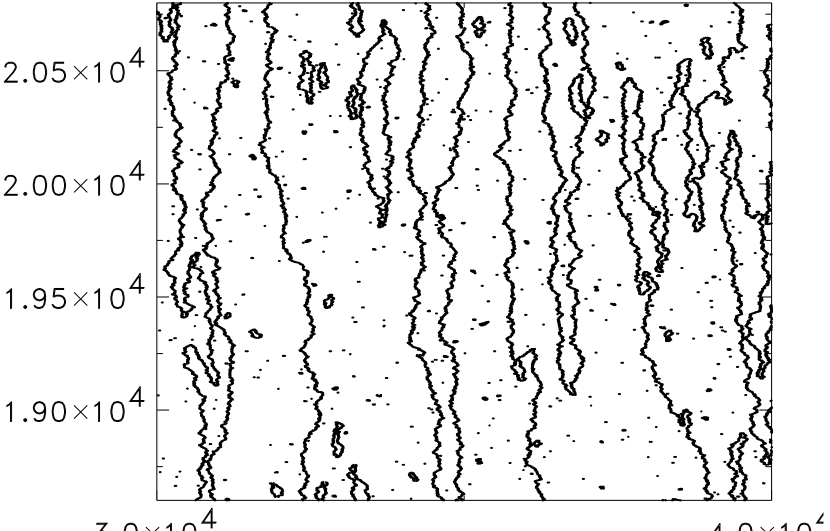
2. Dynamics
   - diffusion-limited reaction
   - width of the nucleated region
   - different dynamics, same stationary density

# Dynamics

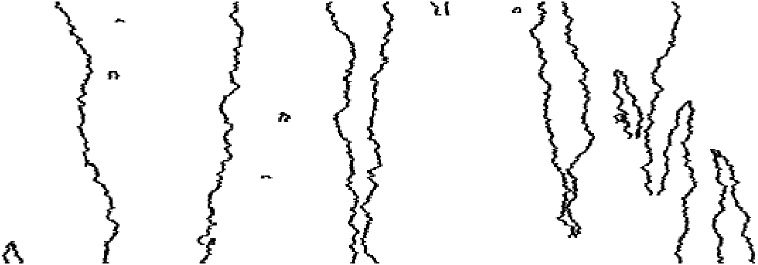
Nucleation . . . Diffusion . . . Annihilation



# Spacetime diagram



# Diffusion-limited reaction: point particles in one dimension



- Particles are nucleated at random times and positions

  in pairs with separation $b$ at rate $\Gamma$

  or

  one at a time at rate $Q$
- Particles diffuse independently with diffusivity $D$
- Particles annihilate on collision.

# Rate equation for unpaired nucleation?

$\rho(t)$ = mean number of particles per unit length.

Exact expressions can be found for $\rho(t)$ and $\rho_\infty = \lim_{t\to\infty} \rho(t)$.

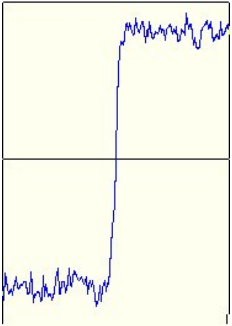

$r(x,t) \equiv$ probability that the number of particles between 0 and $x$ at time $t$ is even.

$$\rho(t) = -\lim_{x\to 0^+} \frac{\partial}{\partial x} r(x,t).$$

$$\text{As } \left(\frac{2\Gamma}{D}\right)^{\frac{1}{3}} b \to 0, \quad \rho_\infty \to \left(\frac{b\Gamma}{2D}\right)^{\frac{1}{2}}.$$

Habib, Lindenberg, Lythe and Molina-París *Diffusion-limited reaction in one dimension: paired and unpaired nucleation* Journal of Chemical Physics **115** 73-89 (2001)

# Kink diffusion coefficient



Part of a configuration that contains only one kink can be decomposed as

$$\mathbf{\Phi}_t(x) = \phi^{\mathrm{k}}(x - \mathbf{X}_t) + \chi_t(x - \mathbf{X}_t).$$

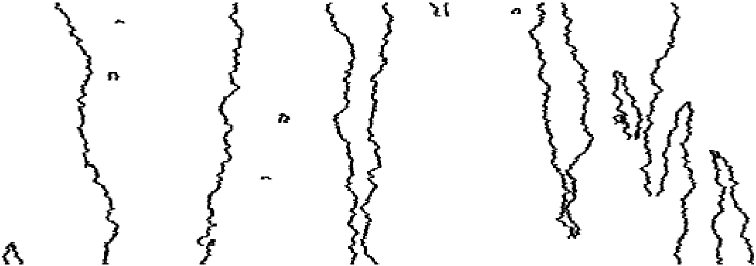
The position, $\mathbf{X}_t$, of an isolated kink undergoes Brownian motion.

Let $D = \lim_{t\to\infty} \frac{1}{2t} \mathbb{E}({\mathbf{X}_t}^2)$. Then $D = \frac{KT}{E_k} + \mathcal{O}((\frac{KT}{E_k})^2)$.


D.J. Kaup
*Thermal corrections to overdamped soliton motion*
Physical Review B **27** 6787-6795 (1983)

GL and Franz Mertens
*Rice's ansatz for overdamped $\phi^4$ kinks at finite temperature*
Physical Review E **67** 027601 (2003)

# Long-term kink dynamics



The density of kinks, $\rho_0$, is proportional to $\exp(-\beta E_k)$.

Nucleation events occur at random spacetime points with rate $\Gamma \propto \exp(-2\beta E_k)$.

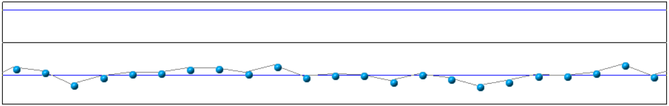
The mean lifetime, $\tau$, of a kink satisfies $\rho_0 = \Gamma\tau$.

Thus the mean lifetime of a kink is proportional to $\exp(\beta E_k)$.

M. Büttiker and T. Christen,
*Diffusion controlled initial recombination*
Physical Review E **58**, 1533 (1998)

# Width of the nucleated region

Using short-to-medium length chains, measure the mean time for whole system to cross from one well to another.



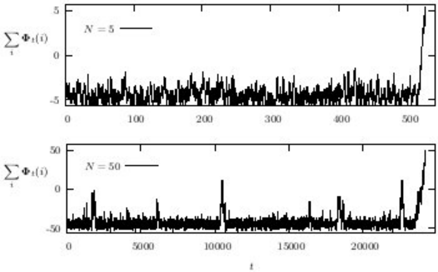
Choose initial condition $\mathbf{\Phi}_0(i) = -1$, $i = 1, \ldots, N$ and denote

$$\mathbf{h} = \inf\{t > 0 : \sum_{i=1}^{N} \mathbf{\Phi}_t(i) = N\}.$$

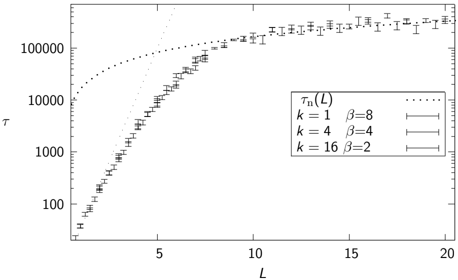
The complete passage time, $\tau$, is the mean of $\mathbf{h}$: $\tau = \mathbb{E}(\mathbf{h})$.

$k = \Delta x^{-2}$ $\quad\quad$ $L = N\Delta x$.

# Collective transition or nucleation-diffusion



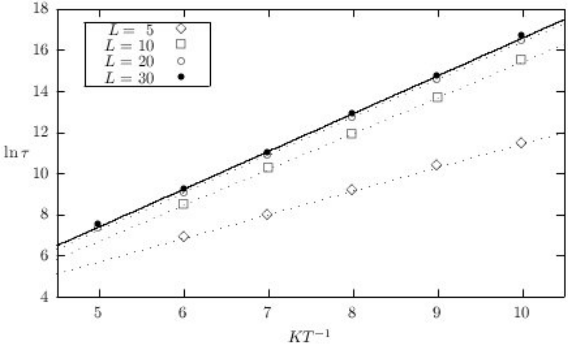

Upper timeseries: $N = 5$, collective regime;
Lower timeseries: $N = 50$, nucleation-diffusion regime.




Complete passage time, $\tau$, as a function of $L$ with $KT = \frac{1}{8}$.

# Width of the nucleated region

$\tau = A(L)\exp(\frac{1}{4KT}f(L))$, where $f(L) \to b$?
We fit numerical results to $\ln\tau = \frac{1}{4KT}b$.




As $L \to \infty$, $f(L) \to b$ where $b = 7.4 \pm 0.1$.
Note: $b = 8E_0$ is consistent with $\Gamma \propto \exp(-2\beta E_k)$.

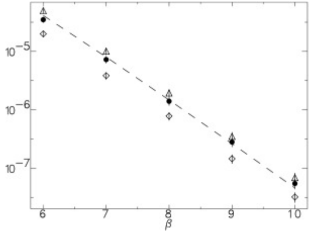

Mario Castro and GL, *Numerical Experiments on Noisy Chains: From Collective Transitions to Nucleation-Diffusion*
SIAM Applied Dynamical Systems **7** 207-219 (2008)

# Kink dynamics when the SPDE is second order in time?

$$\mathrm{d}\mathbf{\Phi}_t(i) = \mathbf{\Pi}_t(i)\mathrm{d}t$$

$$\mathrm{d}\mathbf{\Pi}_t(i) = \left(\mathbf{\Phi}_t(i) - \mathbf{\Phi}_t^3(i) + \mathcal{L}\mathbf{\Phi}_t(i) - \eta\mathbf{\Pi}_t(i)\right)\mathrm{d}t + \left(\frac{2\eta KT}{\Delta x}\right)^{\frac{1}{2}}\mathrm{d}\mathbf{W}_t(i)$$

- The stationary density is independent of $\eta$.
- The nucleation rate is always proportional $\exp(-2\beta E_k)$.




$\eta = 0.2$ (triangles),
$\eta = 1$ (filled circles)
$\eta = 5$ (diamonds)
The solid line is $\Gamma = \rho_k^2$.

- The dynamics is strongly $\eta$-dependent.

Lythe and Habib *Dynamics of kinks: nucleation, diffusion and annihilation*
Physical Review Letters **84** 1070 (2000)