# Breaking the chain

Michael Allman

Mathematics Institute
University of Warwick
Coventry, UK

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PhD supervisor: Volker Betz (Warwick)

# General set-up

Let $\mathbf{x}(s) = (x_0(s), x_1(s), \ldots, x_N(s))$ be the positions of $N+1$ particles in $\mathbb{R}$ at time $s$, evolving according to

$$\mathrm{d}x_i(s) = -\frac{\partial H}{\partial x_i}(\mathbf{x}(s))\,\mathrm{d}s + \sigma \mathrm{d}W_i(s), \quad 0 \leqslant i \leqslant N$$

where $H$ is potential energy of the chain given by

$$H(\mathbf{x}) = \sum_{0 \leqslant i<j \leqslant N} U(x_i - x_j)$$

and $U$ is a pair potential.

Main properties of $U$:

- $U$ has a unique minimum at $a > 0$
- $U$ has finite range $b > 0$
- $b < 2a$

Initially we take the chain to be in the minimal energy configuration:

$$\mathbf{x}(0) = (0, a, 2a, \ldots, Na)$$

We would like to slowly stretch the chain of particles:
Fix $x_0 \equiv 0$ and let $x_N(s) = Na(1 + \varepsilon s)$, where $\varepsilon > 0$ is small.

The other $N-1$ particles then evolve according to

$$\mathrm{d}x_i(s) = -\frac{\partial H}{\partial x_i}(\mathbf{x}(s), \varepsilon s)\,\mathrm{d}s + \sigma \mathrm{d}W_i(s), \;\; 1 \leqslant i \leqslant N-1$$

where $H$ is now the time-dependent potential energy of the chain given by

$$H(\mathbf{x}, \varepsilon s) = \sum_{0 \leqslant i<j \leqslant N-1} U(x_i - x_j) + \sum_{0 \leqslant i \leqslant N-1} U(x_i - Na(1+\varepsilon s))$$

As the chain is stretched, new minimal energy configurations will become possible.

We consider the chain to break when its configuration enters a small neighbourhood of one of these new minima.

We define the break location by which of the new minima is reached first.

General goal: Writing $\varepsilon = \varepsilon(\sigma)$, to identify how different speeds of stretching affect the break location, as $\sigma \downarrow 0$.

# Three particles

Take $N = 3$ so that $\mathbf{x}(s) = (0, x_s, 2a(1 + \varepsilon s))$.
Only the middle particle is free. It satisfies a one-dimensional non-autonomous SDE

$$\mathrm{d}x_s = -\frac{\partial H}{\partial x}(x_s, \varepsilon s)\mathrm{d}s + \sigma \mathrm{d}W_s$$

with initial condition $x_0 = a$ and time-dependent potential energy given by

$$H(x, \varepsilon s) = U(x) + U(2a(1 + \varepsilon s) - x)$$

We rescale time as $t = \varepsilon s$, so that $\mathbf{x}(t) = (0, x_t, 2a(1+t))$ and $x_t$ solves

$$\mathrm{d}x_t = -\frac{1}{\varepsilon}\frac{\partial H}{\partial x}(x_t, t)\mathrm{d}t + \frac{\sigma}{\sqrt{\varepsilon}}\mathrm{d}W_t$$

We say the chain breaks as soon as the middle particle is a distance $b$ from one of its neighbours.

So the chain is unbroken at time $t$ if

$$x_t < b \quad \text{and} \quad 2a(1+t) - x_t < b$$

which combine to give

$$2a(1+t) - b < x_t < b$$

Let

$$\tau = \inf\{t \geqslant 0 : x_t \notin (2a(1+t) - b, b)\}$$

This is the time that the chain breaks. Clearly,

$$\tau \leqslant b/a - 1$$

so the chain breaks in finite time.

The chain breaks on the left-hand side if $x_\tau = b$.

Otherwise, it breaks on the right-hand side.

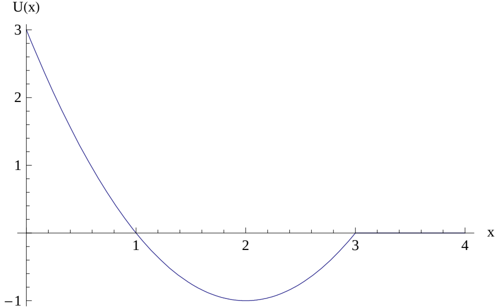
Recall that our potential $U$ has unique minimum at $a > 0$ and finite range $b > 0$, where $b < 2a$. In addition, we will assume:

There exists $a_0 \in (0, a)$ such that $U''(y) \geqslant u_0 > 0$ for all $y \in (a_0, b)$.

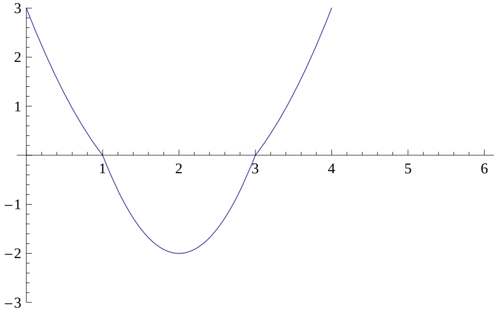
An example of such a potential is a cut-off quadratic given by

$$U(y) = \begin{cases} (|y| - a)^2 - (b - a)^2 & 0 \leqslant |y| \leqslant b \\ 0 & \text{otherwise} \end{cases}$$

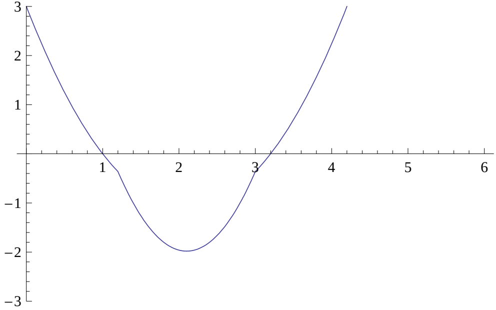
where $b < 2a$, shown below for $a = 2, b = 3$.



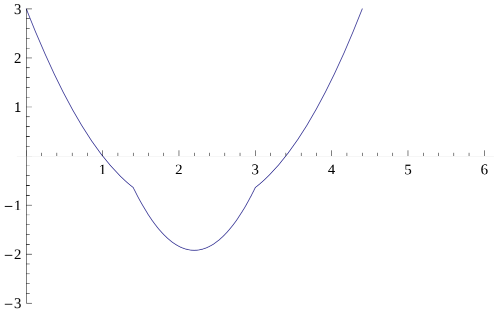
The potential energy $H(x,t) = U(x) + U(2a(1+t) - x)$ when $t = 0$



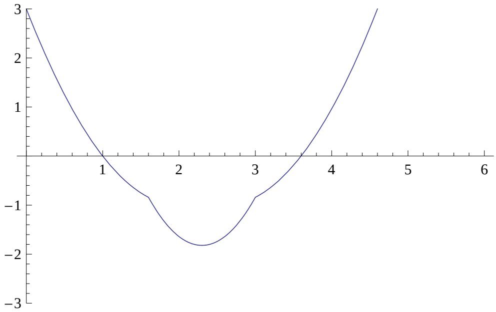
## $t = 0.05$



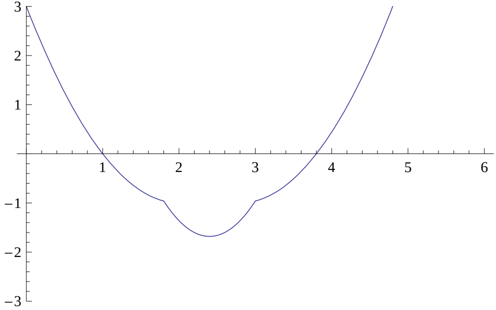
$t = 0.1$



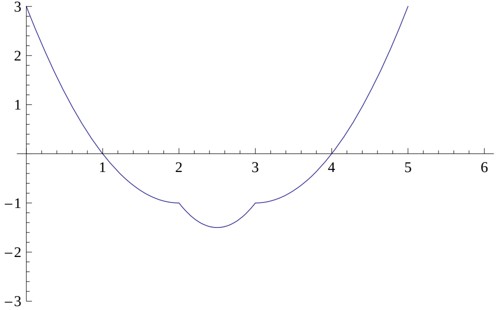
$t = 0.15$



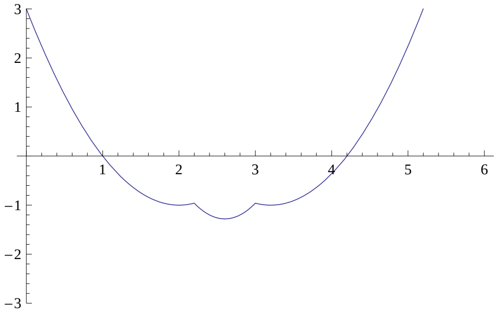
## $t = 0.2$



$t = 0.25$



$t = 0.3$



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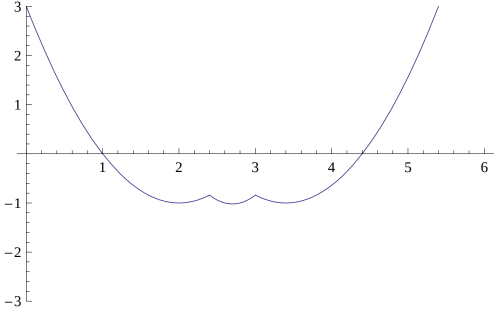
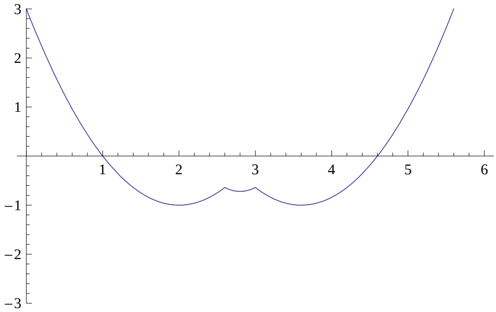
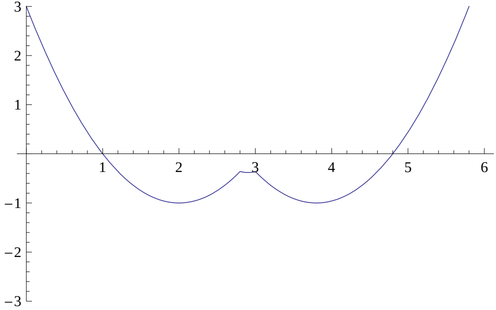


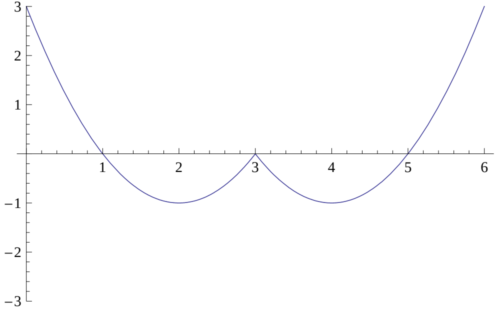
$t = 0.4$



$t = 0.45$



$t = 0.5$



Notation: $f(\sigma) \ll g(\sigma)$ means $f(\sigma)/g(\sigma) \to 0$ as $\sigma \downarrow 0$.

## Theorem (A.,Betz)

1. *Fast Stretching*
   *If*
   $$\sigma |\ln \sigma|^{1/2} \ll \varepsilon(\sigma) \ll 1$$
   *then* $\mathbb{P}\{x_\tau = b\} \to 0$ *as* $\sigma \downarrow 0$.
2. *Slow Stretching*
   *If*
   $$\frac{1}{\sigma^{2/3}} \exp\left\{-\frac{1}{\sigma^{2/3}}\right\} \ll \varepsilon(\sigma) \ll \sigma |\ln \sigma|^{-1/2}$$
   *then* $\mathbb{P}\{x_\tau = b\} \to 1/2$ *as* $\sigma \downarrow 0$.

In the slow stretching case, we expect the result to hold without the lower bound on $\varepsilon$, i.e. for all

$$\varepsilon \ll \sigma |\ln \sigma|^{-1/2}$$

Indeed, when $U$ is quadratic, this is true.

The lower bound is related to the theory of large deviations.

# Deterministic Dynamics

Let $x_t^{\text{det}}$ be solution when $\sigma = 0$,

$$\frac{\mathrm{d}}{\mathrm{d}t} x_t^{\text{det}} = -\frac{1}{\varepsilon}\frac{\partial H}{\partial x}(x_t^{\text{det}}, t)$$

with $x_0^{\text{det}} = a$. A particular solution is given by

$$x_t^{\text{det}} = a(1+t) - \frac{\varepsilon a}{2U''(a(1+t))} + \mathcal{O}(\varepsilon^2)$$

This shows $x_t^{\text{det}}$ lags behind the midpoint of the chain at distance $\mathcal{O}(\varepsilon)$. So the deterministic chain always breaks on the right-hand side.

We expect $x_t$ to stay close to $x_t^{\text{det}}$. Let

$$y_t = x_t - x_t^{\text{det}}$$

For the chain to be unbroken, we require

$$2a(1+t) - b < x_t < b$$

which is the same as

$$2a(1+t) - b - x_t^{\text{det}} < y_t < b - x_t^{\text{det}}$$

Using our expression for $x_t^{\text{det}}$, this gives

$$a(1+t) - b + \mathcal{O}(\varepsilon) < y_t < b - a(1+t) + \mathcal{O}(\varepsilon)$$

where the $\mathcal{O}(\varepsilon)$ terms are both the same and are uniform in $t$.

Then the breaking time, $\tau$, can be expressed in terms of $y_t$:

$$\tau = \inf\{t \geqslant 0 : y_t \notin (d_-(t), d_+(t))\}$$

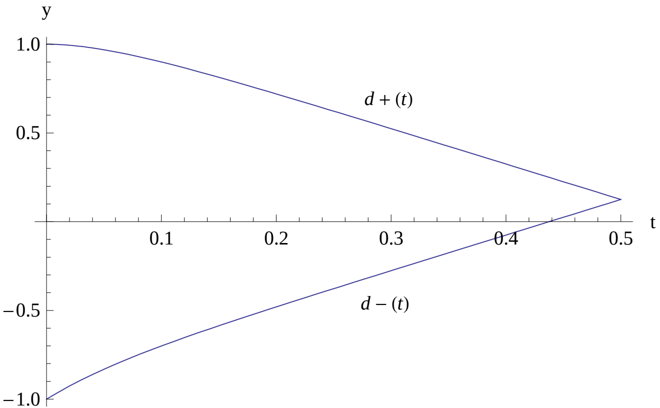
where

$$d_+(t) = b - x_t^{\text{det}} = b - a(1+t) + \mathcal{O}(\varepsilon)$$

and

$$d_-(t) = 2a(1+t) - b - x_t^{\text{det}} = a(1+t) - b + \mathcal{O}(\varepsilon)$$

Now, the chain breaks on the left-hand side if $y_\tau = d_+(\tau)$.



y
1.0
0.5
−0.5
−1.0
0.1
0.2
0.3
0.4
0.5
t
d + (t)
d − (t)

We would like to show that $y_t$ never gets too big. The following lemma is based on a result by Berglund and Gentz.

**Lemma**

*Let* $\sigma \ll D(\sigma) \ll 1$ *be such that*

$$\frac{D^2}{\sigma^2} \exp\left\{-\frac{D^2}{\sigma^2}\right\} \ll \varepsilon(\sigma) \ll 1$$

*Then*

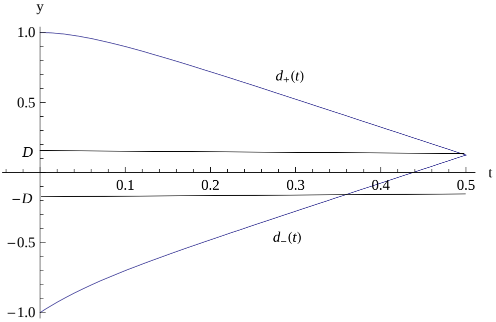
$$\lim_{\sigma \downarrow 0} \mathbb{P}\left\{\sup_{0 \leqslant t \leqslant \tau} |y_t| \geqslant D\right\} = 0$$

The lower bound on $\varepsilon$ is related to the Eyring-Kramers time.

An excursion of size $D$ corresponds to climbing a potential height of $\mathcal{O}(D^2)$, which we expect to occur as soon as $t/\varepsilon$ is of order $\mathrm{e}^{D^2/\sigma^2}$.

# Fast Stretching

When $\sigma|\ln\sigma|^{1/2} \ll \varepsilon(\sigma) \ll 1$, we can use the lemma with $D = d_+(b/a - 1)$ to show that $|y_t| < d_+(b/a - 1)$ for all $0 \leqslant t \leqslant \tau$.



# Slow Stretching

The process $y_t$ can be written

$$y_t = y_t^0 + y_t^1$$

where $y_t^0$ is a centred Gaussian process with variance $\mathcal{O}(\sigma^2)$ and $y_t^1$ satisfies

$$|y_t^1| \leqslant C \sup_{0 \leqslant s \leqslant t} y_s^2$$

Given $D$ such that

$$\lim_{\sigma \downarrow 0} \mathbb{P}\left\{ \sup_{0 \leqslant t \leqslant \tau} |y_t| \geqslant D \right\} = 0$$

we can assume that for all $0 \leqslant t \leqslant \tau$,

$$y_t^0 - D^2 \leqslant y_t \leqslant y_t^0 + D^2$$

since all other cases have zero probability as $\sigma \downarrow 0$.

Then

$$\mathbb{P}\{y_\tau = d_+(\tau)\} \leqslant \mathbb{P}\{y_t^0 + D^2 \text{ hits } d_+(t) \text{ before } d_-(t)\}$$

and

$$\mathbb{P}\{y_\tau = d_+(\tau)\} \geqslant \mathbb{P}\{y_t^0 - D^2 \text{ hits } d_+(t) \text{ before } d_-(t)\}$$

We must show that the upper and lower bounds tend to $1/2$.

To show

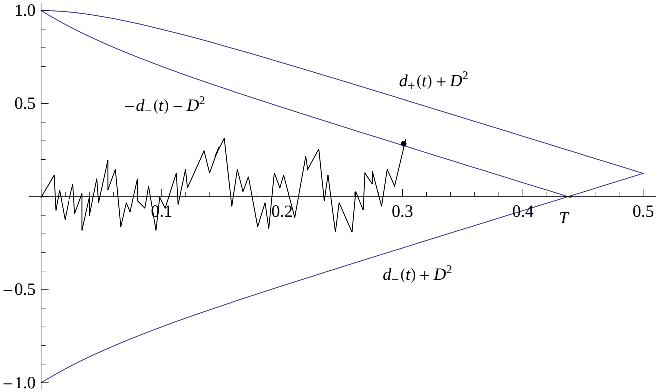
$$\lim_{\sigma \downarrow 0} \mathbb{P}\{y_t^0 - D^2 \text{ hits } d_+(t) \text{ before } d_-(t)\} = 1/2$$

we first rewrite it as

$$\lim_{\sigma \downarrow 0} \mathbb{P}\{y_t^0 \text{ hits } d_+(t) + D^2 \text{ before } d_-(t) + D^2\} = 1/2$$

We know that $y_t^0$ has an entirely symmetric distribution, so we first consider the stopping time given by

$$\tau_L = \tau_L(D) = \inf\{t \geqslant 0 : |y_t^0| \geqslant -d_-(t) - D^2\}$$


1.0
0.5
−0.5
−1.0
0.1
0.2
0.3
0.4
0.5
T
$d_+(t) + D^2$
$-d_-(t) - D^2$
$d_-(t) + D^2$

We need information about the distribution of $\tau_L$.

Roughly speaking, we show that $\tau_L$ is concentrated near $b/a - 1 - \sigma$.

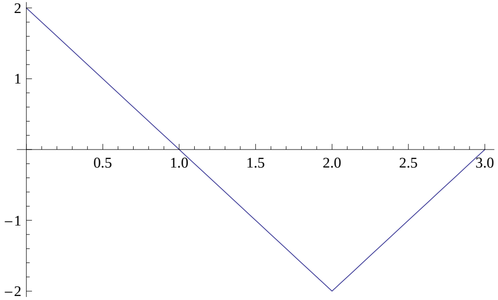
We then show that if

$$y^0_{\tau_L} = -d_-(\tau_L) - D^2$$

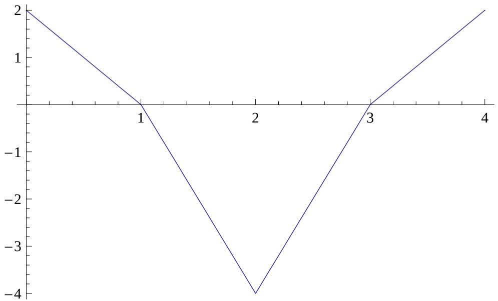
then $y^0_t$ hits $d_+(t) + D^2$ soon after, by picking a suitable interval $[\tau_L, \tau_L + \Delta]$ and applying the reflection principle.

# Comparison with a linear potential

Suppose $U$ is piecewise linear, as below.



The potential energy $H(x,t) = U(x) + U(2a(1+t) - x)$ when $t = 0$



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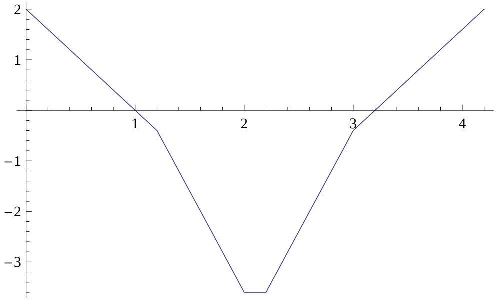
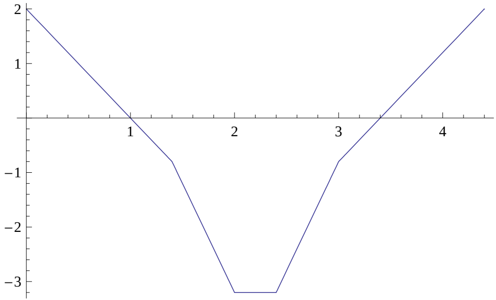


## $t = 0.1$



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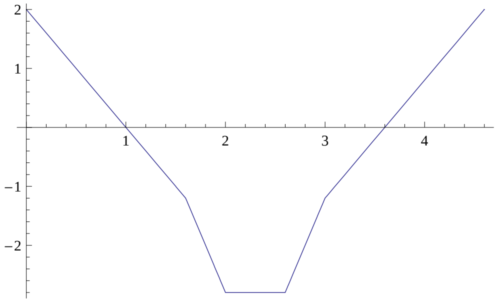
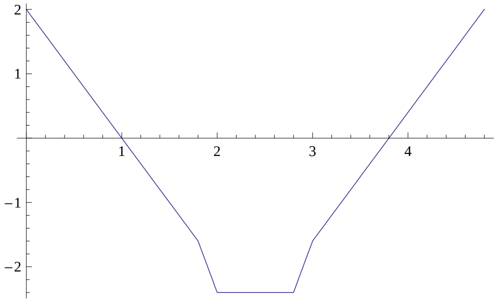
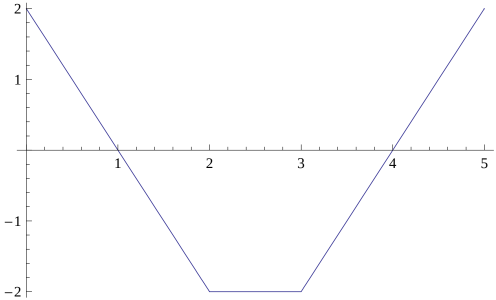


$t = 0.2$



$t = 0.25$



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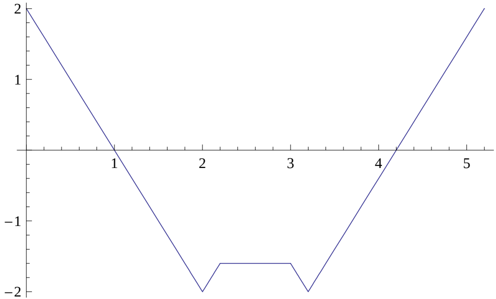

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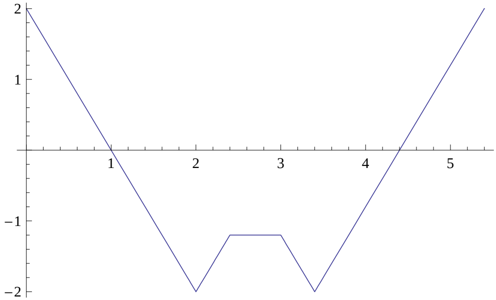

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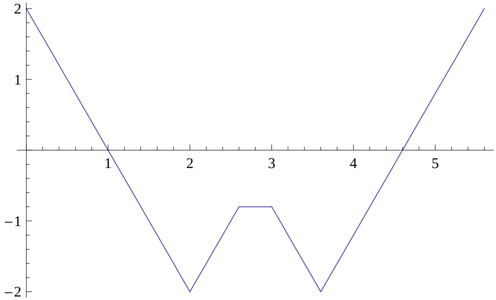

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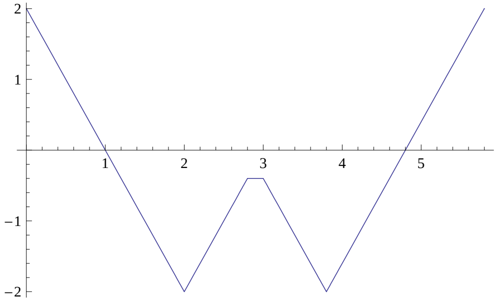

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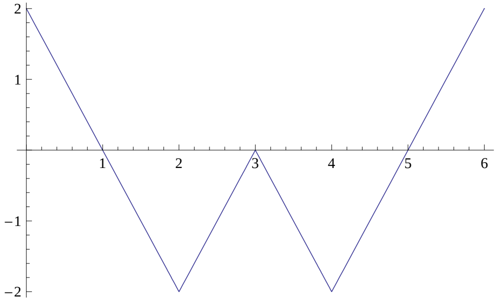


When $x$ is near the middle of the chain, it moves like free Brownian motion:

$$x_t = \frac{\sigma}{\sqrt{\varepsilon}} W_t$$

with no drift term making it follow the midpoint of the chain. Recall that the chain is unbroken if $x_t$ satifies

$$2a(1+t) - b < x_t < b$$

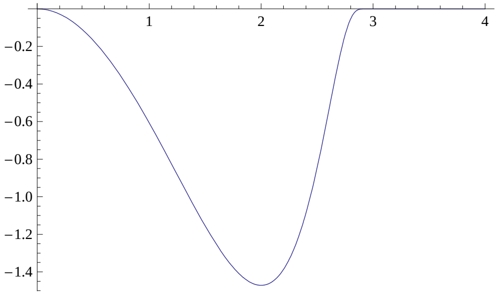
To behave non-deterministically, $x_t$ must diffuse with speed $\mathcal{O}(1)$. We see that $\sigma = \varepsilon^{1/2}$ is the critical scaling.

Hence, we require stronger noise to cause non-deterministic behaviour.

# Next step

We want to do the same with $U$ differentiable everywhere.
Example:

$$U(y) = \begin{cases} -y^2\,\mathrm{e}^{-1/(3-y)} & 0 \leqslant |y| \leqslant 3 \\ 0 & \text{otherwise} \end{cases}$$



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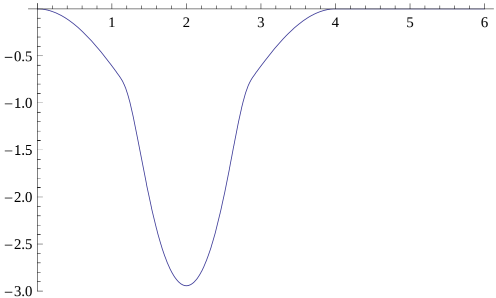

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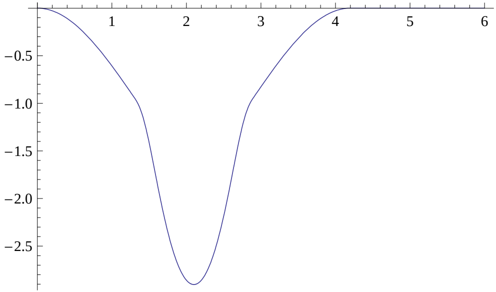
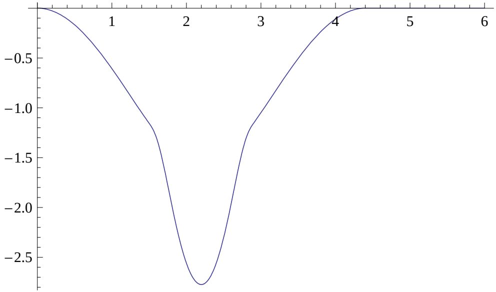


## $t = 0.1$



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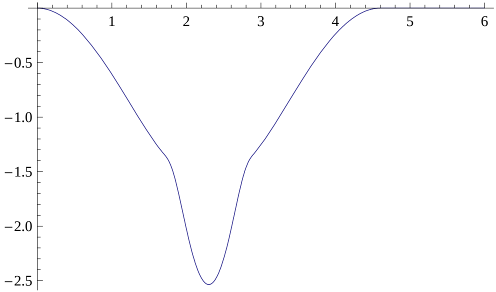

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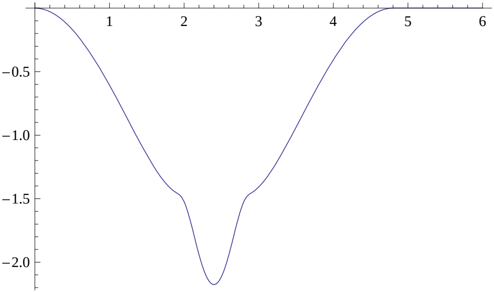

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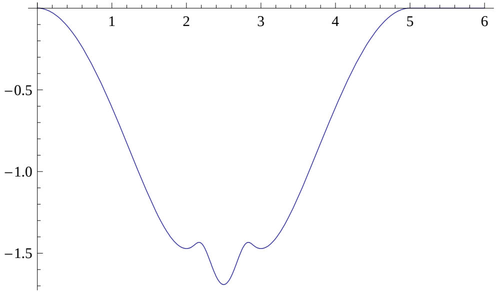

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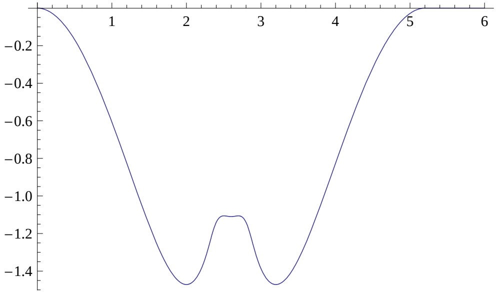

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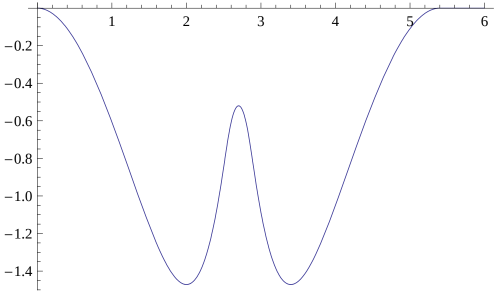

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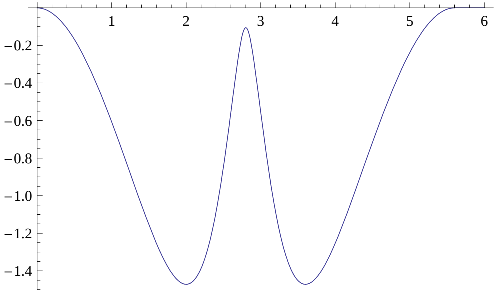

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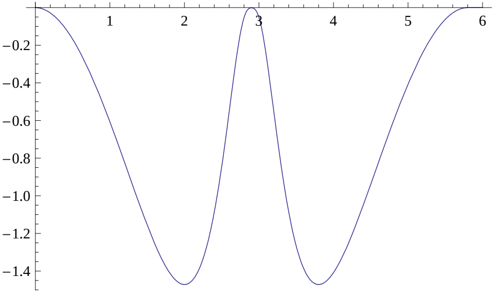

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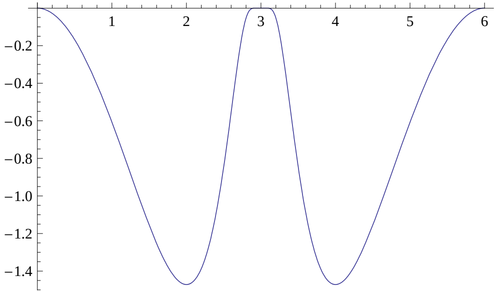

# Deterministic Dynamics

Let

$$z_t = a(1+t) - x_t^{\text{det}}$$

Assuming that there is a unique $x_0 \in (a,b)$ such that $U''(x_0) = 0$, we can show there are constants $c_1, c_2 > 0$ such that

$$z_t \asymp \begin{cases} \varepsilon/(T-t) & 0 \leqslant t \leqslant T - c_1\varepsilon^{1/2} \\ \varepsilon^{1/2} & T - c_1\varepsilon^{1/2} \leqslant t \leqslant T + c_2\varepsilon^{1/2} \end{cases}$$

where $T$ is the time bifurcation occurs at midpoint.

Again we let

$$y_t = x_t - x_t^{\text{det}}$$

and write it as $y_t = y_t^0 + y_t^1$. Then the variance of $y_t^0$ behaves like

$$\mathrm{Var}(y_t^0) \asymp \begin{cases} \sigma^2/(T-t) & 0 \leqslant t \leqslant T - c_1\varepsilon^{1/2} \\ \sigma^2\varepsilon^{-1/2} & T - c_1\varepsilon^{1/2} \leqslant t \leqslant T + c_2\varepsilon^{1/2} \end{cases}$$

If the typical spreading of $y_t^0$ is bigger than $z_t$, then we expect equal chance to break on either side. Here, we require

$$\sigma\varepsilon^{-1/4} \gg \varepsilon^{1/2}$$

That is, we require $\sigma \gg \varepsilon^{3/4}$ .