Asymptotic velocity of one dimensional diffusions with periodic drift.

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We wanted to understand if these models really work.

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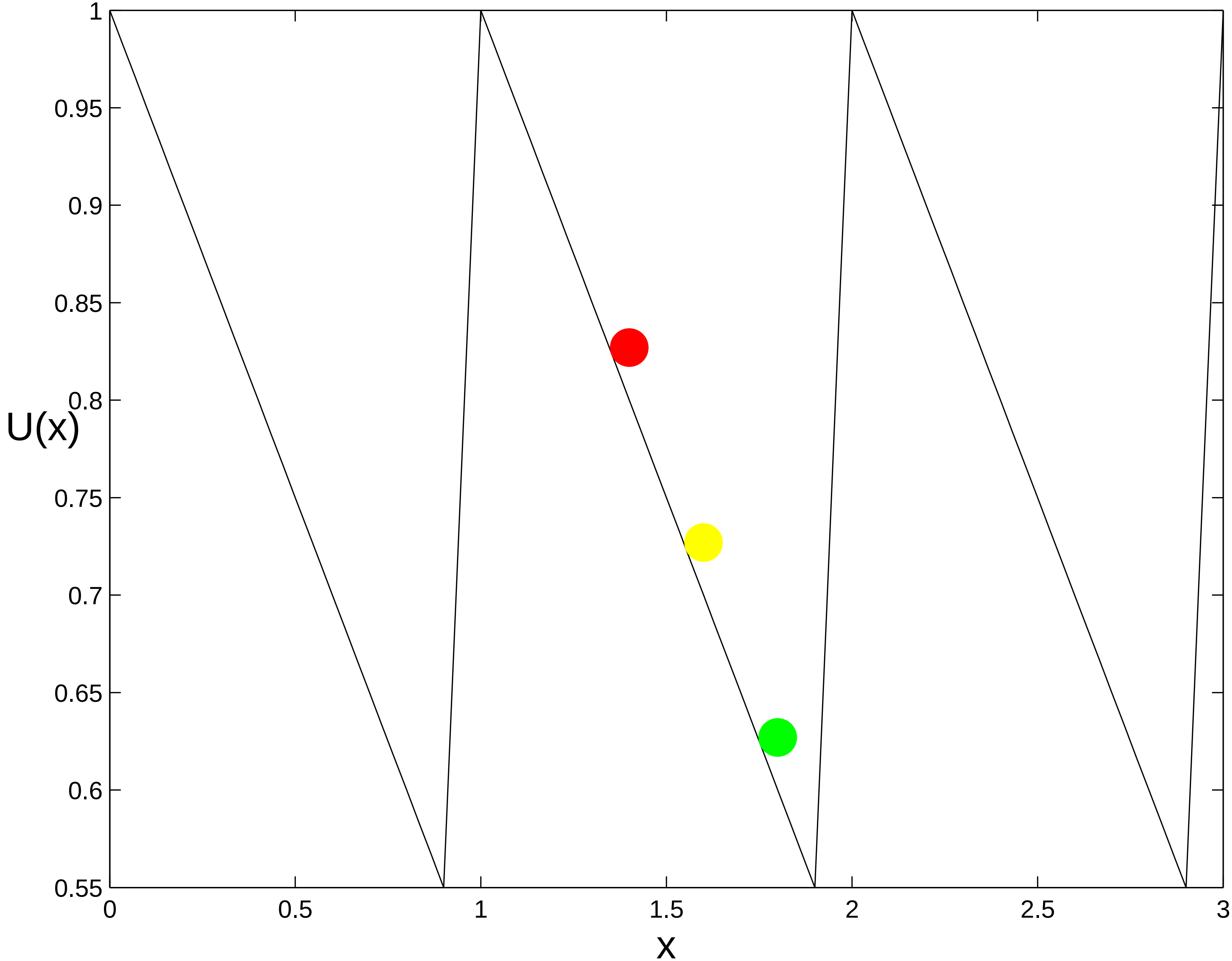
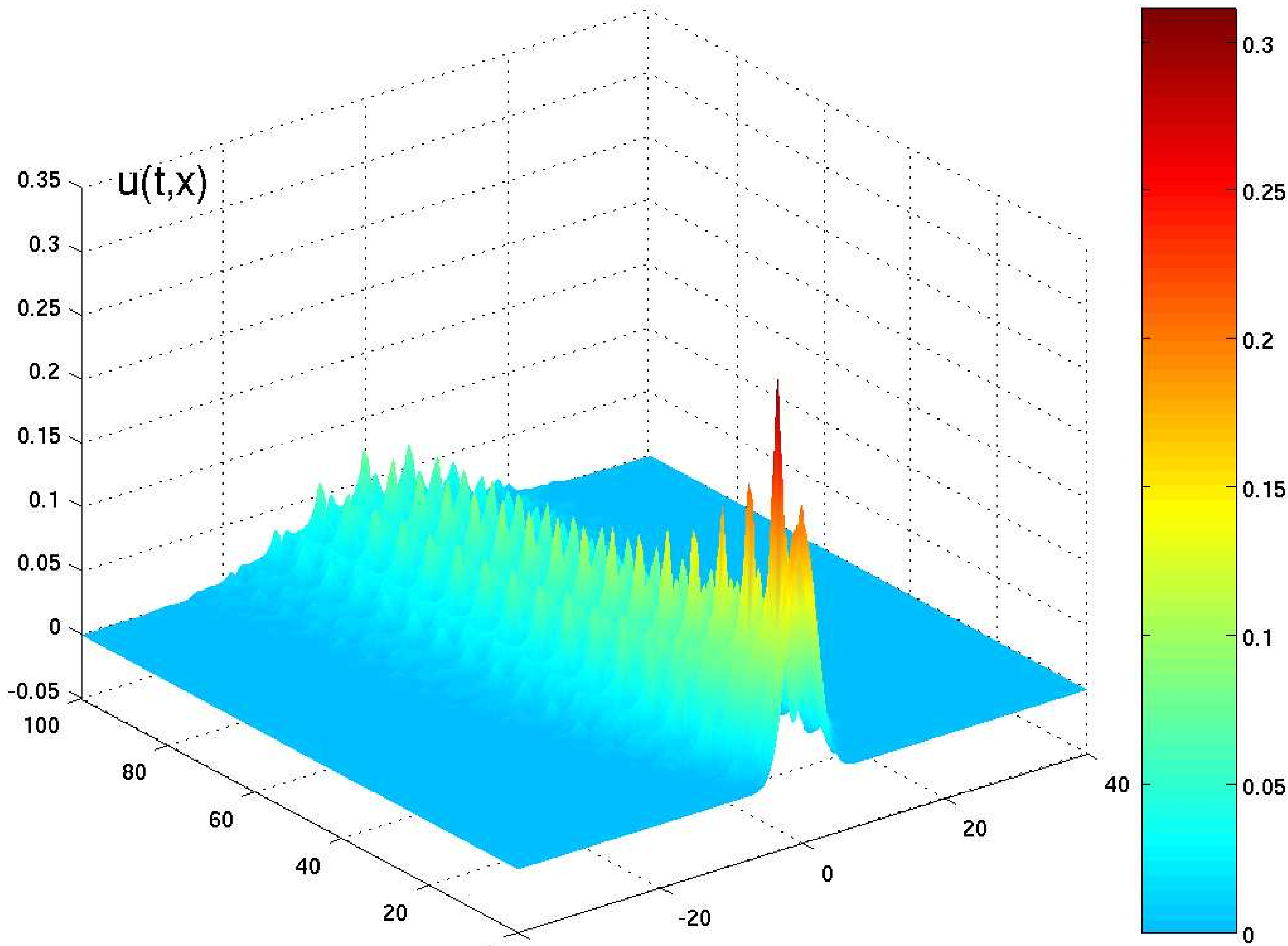
During a part of the period the potential is zero (constant) and the particles diffuse freely.
In the rest of the period, the potential “concentrates” the particles in its minima.

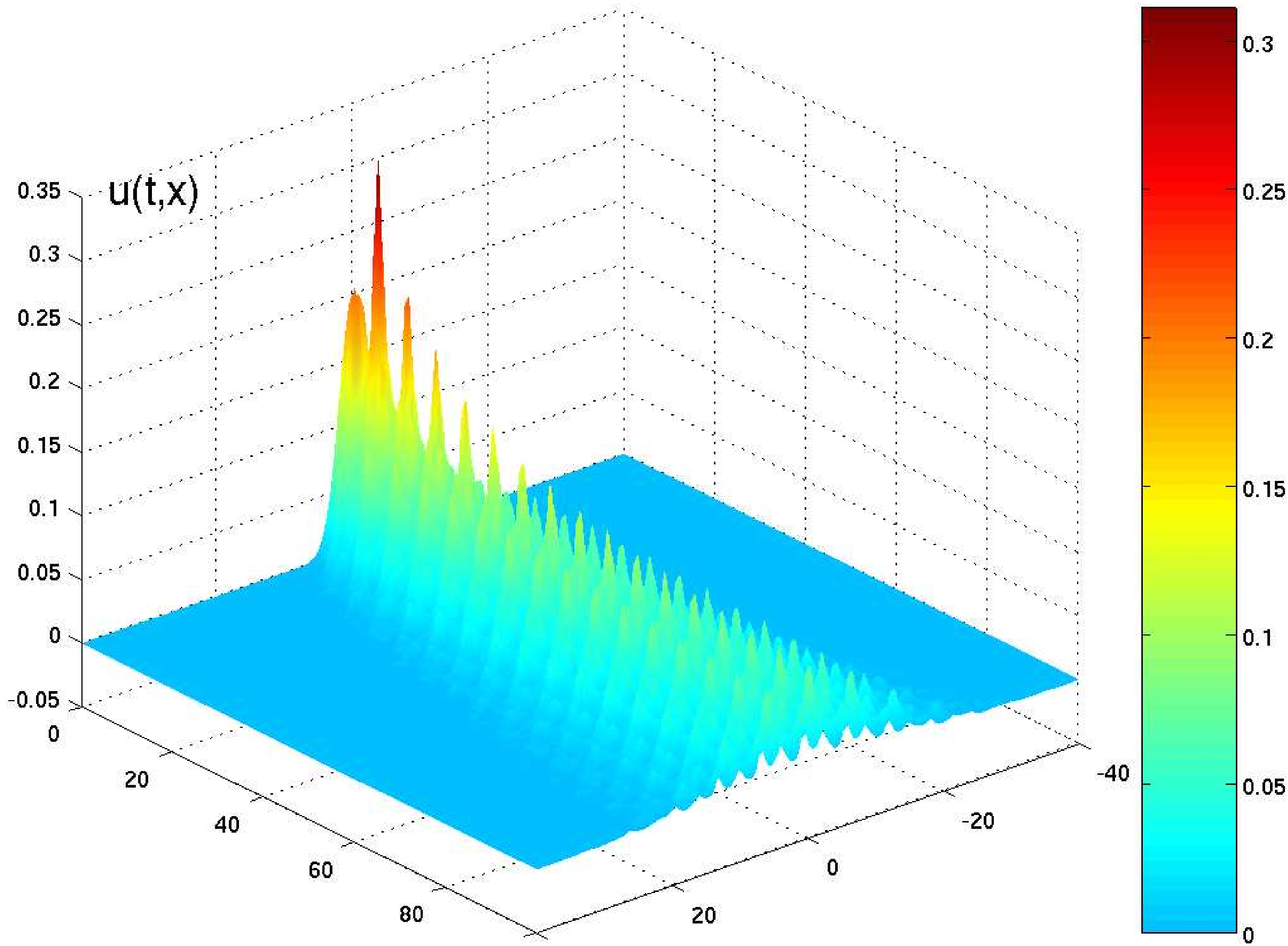
A "simple" model

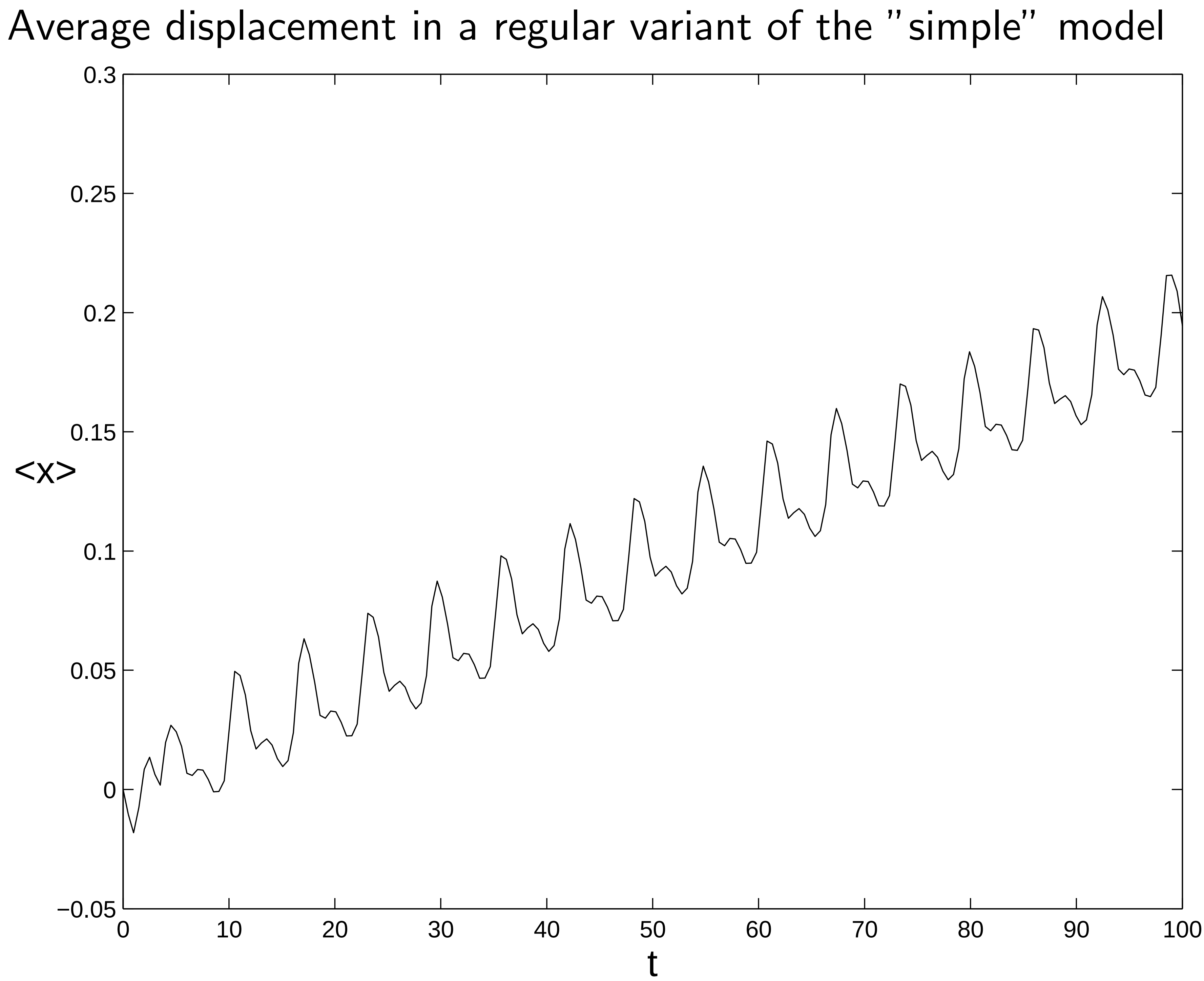


Evolution of the probability density in a regular variant of the "simple" model



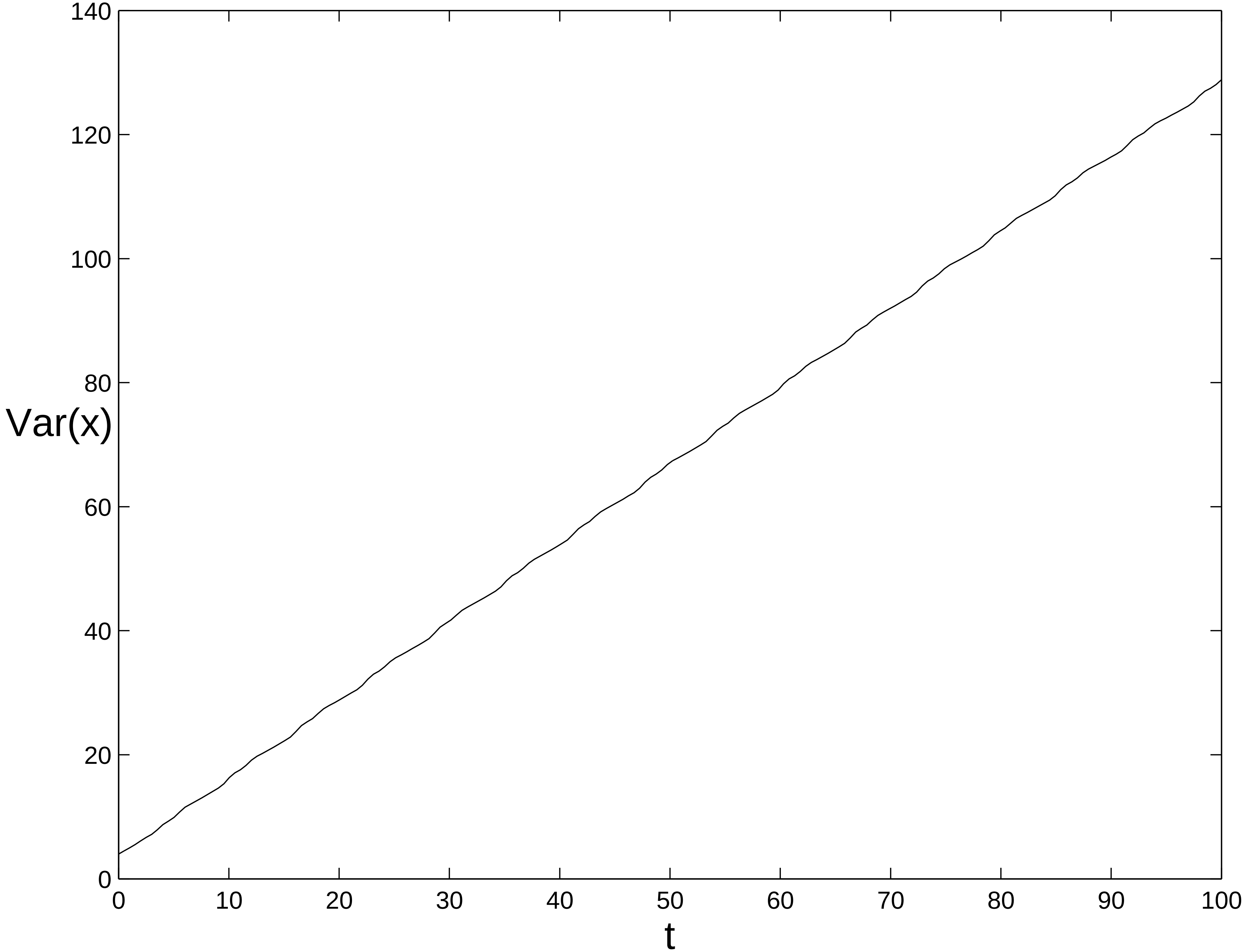
Evolution of the probability density in a regular variant of the "simple" model (backward view)





Average displacement in a regular variant of the "simple" model
0.3
0.25
0.2
0.15
0.1
0.05
0
−0.05
<x>
0
10
20
30
40
50
60
70
80
90
100
t

Variance of the displacement in a regular variant of the "simple" model



These pictures were produced with a potential

$$U(t,x) = -\big(0.5071\ \sin(x + 2.9705) + 0.1351\ \sin(2x + 2.8597)\big)$$

$$\times\ \big(0.3574\ \cos(t - 0.0316) + 0.4956\ \cos(2t + 2.3379)\big)$$

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We have studied four models in dimension one.

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$$\frac{1}{T} \int_0^T b(t, x)\, dt = 0$$

for all x. This is not true in the "simple" model, but holds for the potential used to generate the pictures.

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In other words, if $u(t, x)$ denotes the probability density of the position of the particle at time t, we have

$$\partial_t u(t, x) = \frac{D}{2}\partial_x^2 u(t, x) + \partial_x\big(b(t, x)u(t, x)\big) \ .$$

$D = \sigma^2$ (Fokker-Planck, direct Kolmogorov equation).

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We define the quantity $I(b)$ (asymptotic displacement per unit of time) by

$$I(b) = \lim_{t\to\infty} \frac{1}{t}\mathbb{E}\big(X(t)\big) = \lim_{t\to\infty} \frac{1}{t}\int_{\mathbb{R}} x \ u(t,x) \ dx \ ,$$

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We have put the constraints of the zero averages both in space and time. This imposes more constraints for a working motor.

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The functional $b \mapsto I(b)$ *is (real) analytic and non trivial on* $C^1_{per}(\mathbb{R} \times \mathbb{R})$. *It does not depend on the initial distribution (in* $L^1((1+|x|)dx) \cap C^0_b(\mathbf{R})$*).*

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But there are some.

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However, the set $\left\{ b \,\middle|\, I(b) \neq 0 \right\}$ is open (and dense).

Therefore if we have a working motor, perturbations not too large will also lead to a working motor in the same direction (perhaps with slightly different speed). This stability is probably important in Biology.

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Integrating over other time intervals of one period give conjugated diffeomorphisms.

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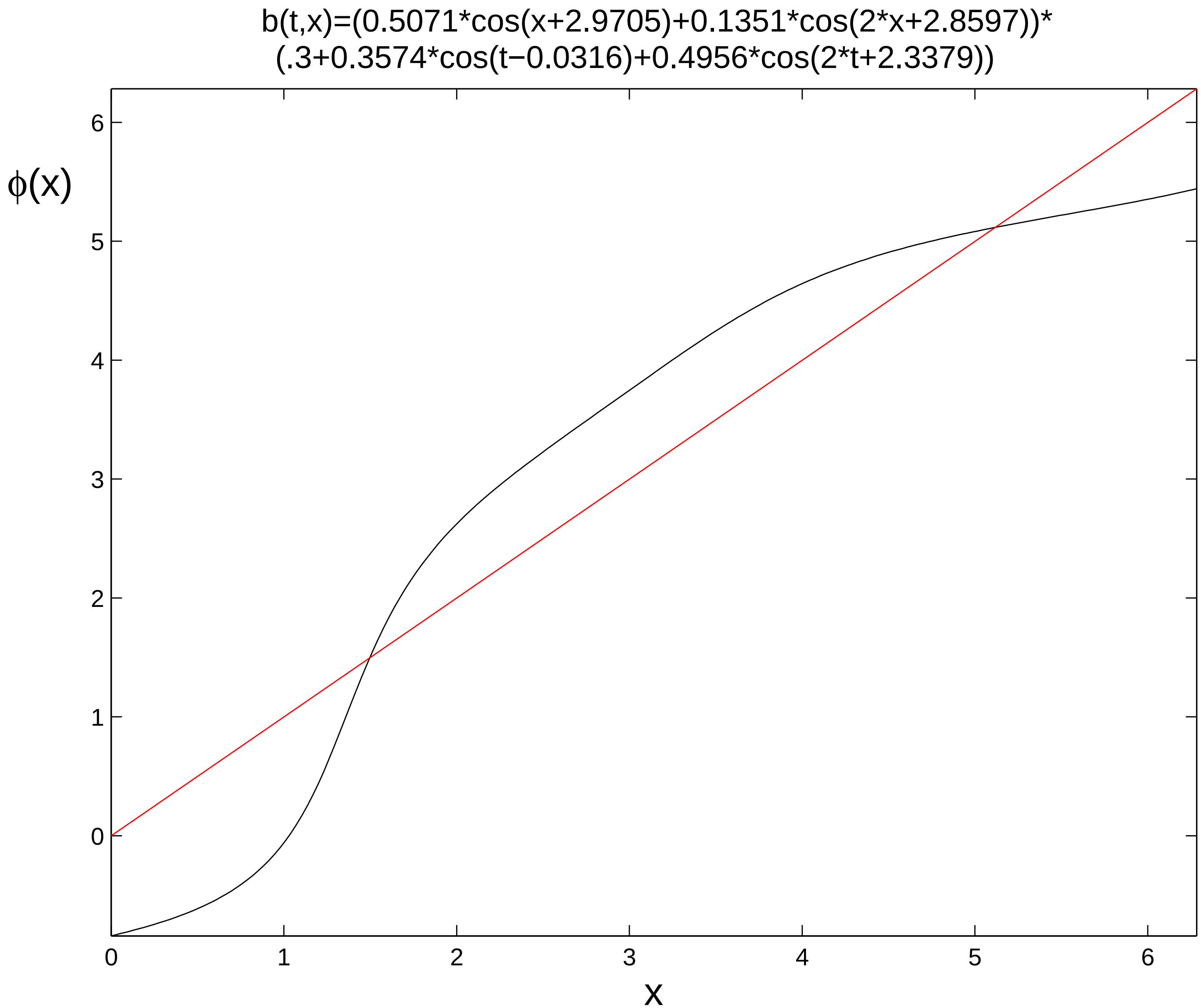
If the slope of the diffeomorphism at the fixed point does not vanish, then there is an open set of b where $\rho = 0$ (stability of hyperbolic fixed points).

An example with rotation number equal to zero (stable)



note that the average over time (at fixed x) is not zero.

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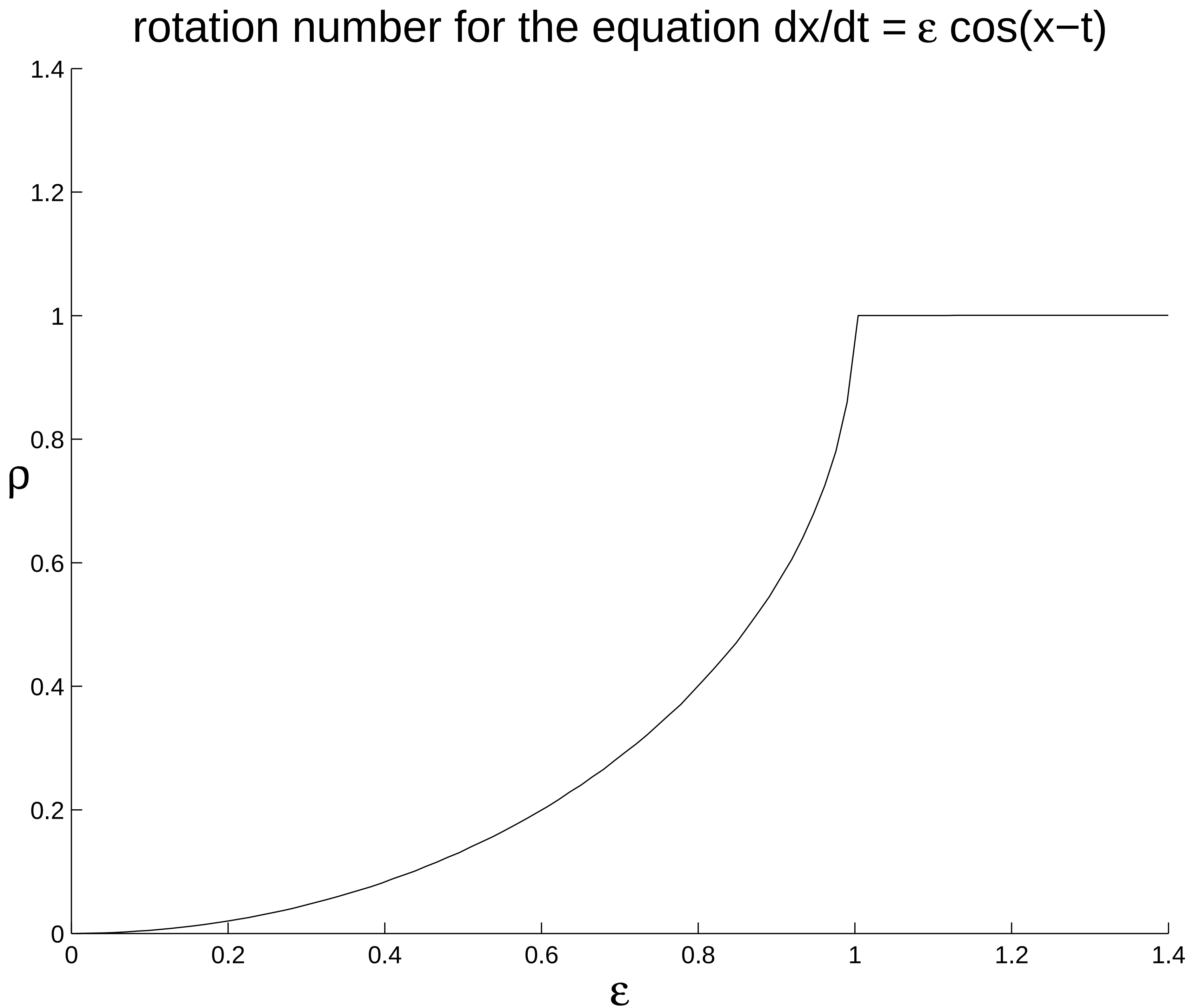
Waves can lead to working motors with no noise

$$\frac{dx}{dt} = \varphi(x - ct)$$

where φ is periodic of zero average.

Velocity of a simple “wave” potential



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An analytic function is either constant or non-trivial. In this second case, the complement of the zero set (analytic set) is open and dense (generic, prevalent).

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$$I(b) = -\frac{1}{T}\int_0^T \int_0^L b(t,x)\, w_b(t,x)\, dt\, dx$$

where $w_b(t,x)$ is periodic in t and x, of integral one in x (independent of t) and satisfies

$$\partial_t w_b(t,x) = \partial_x\left(\frac{D}{2}\partial_x w_b(t,x) + b(t,x) w_b(t,x)\right)\ .$$

There exists a unique such function (this is related to Floquet multipliers).

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$$b(t,x) = \sum_{p,q} b_{p,q} e^{2\pi i (pt/T + qx/L)} \ .$$

Recall that b should be real, hence $\overline{b_{p,q}} = b_{-p,-q}$. Also $b_{0,p} = 0$ and $b_{q,0} = 0$ (vanishing space and time averages).

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$$I(b) = \sum_{p,q} \frac{p\, q L^3 T^2}{p^2 L^4 + \pi^2 q^4 T^2} \left| b_{p,q} \right|^2 + \mathcal{O}(b^3) \ .$$

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This gives an idea of the zero set of I near $b = 0$.

A more realistic model (model II).

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Chemical reactions take place which modify the state of the substrate, hence modifying the interaction of the particle with the substrate.
In a better model based on the biochemistry inside the cells, the substrate can be in two states.
At time goes on, the the substrate flips randomly between the two states.

We denote by $\rho_1(t, x)$ the probability density that the molecule is at position x at time t and the substrate is in state one. We denote similarly $\rho_2(t, x)$ for state 2.

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The evolution equations are given by

$$\begin{aligned}
\partial_t \rho_1 = &\quad \partial_x \big(\mathscr{D} \partial_x \rho_1 + b_1(x)\rho_1\big) - \nu_1 \rho_1 + \nu_2 \rho_2 \\
\partial_t \rho_2 = &\quad \partial_x \big(\mathscr{D} \partial_x \rho_2 + b_2(x)\rho_2\big) + \nu_1 \rho_1 - \nu_2 \rho_2
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\end{aligned}
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$\mathscr{D}$, ν_1 and ν_2 are positive constants. The functions b_1 and b_2 are C^1 periodic functions of x of period L with average zero, independent of time.

The asymptotic average displacement per unit time of the particle is now defined by

$$I(\nu_1, \nu_2, b_1, b_2) = \lim_{t\to\infty} \frac{1}{t} \int x \left(\rho_1(t,x) + \rho_2(t,x)\right) dx \; .$$

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We have a result similar to the case of model I.

Theorem 2

For any constants $\nu_1 > 0$ and $\nu_2 > 0$, and for any b_1 and b_2 $\in C^1_{per}(\mathbb{R})$, the number $I(\nu_1,\nu_2,b_1,b_2)$ is independent of the non negative initial distributions $\rho_1(0,x)$ and $\rho_2(0,x)$ in $L^1((1+|x|)dx)\cap C^0_b(\mathbb{R})$. The set of b_1 and $b_2 \in C^1_{per}(\mathbb{R})$ with space average equal to zero where $I(\nu_1,\nu_2,b_1,b_2)\neq 0$ is open and dense.

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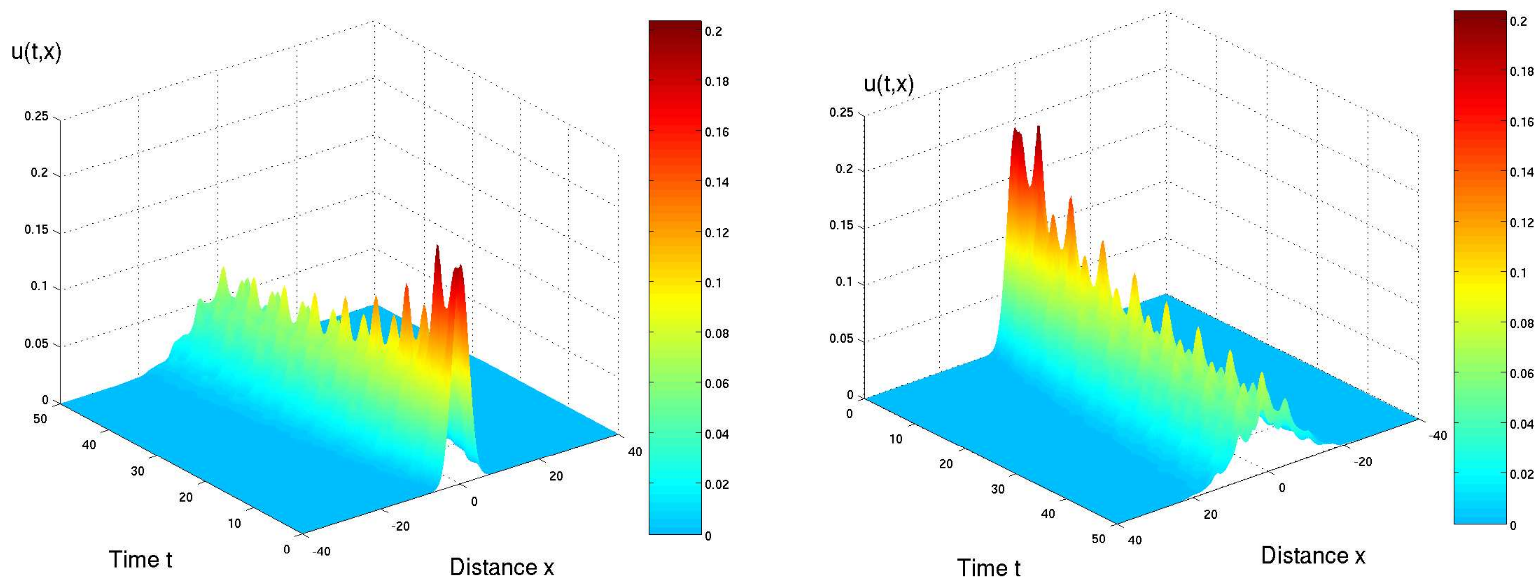
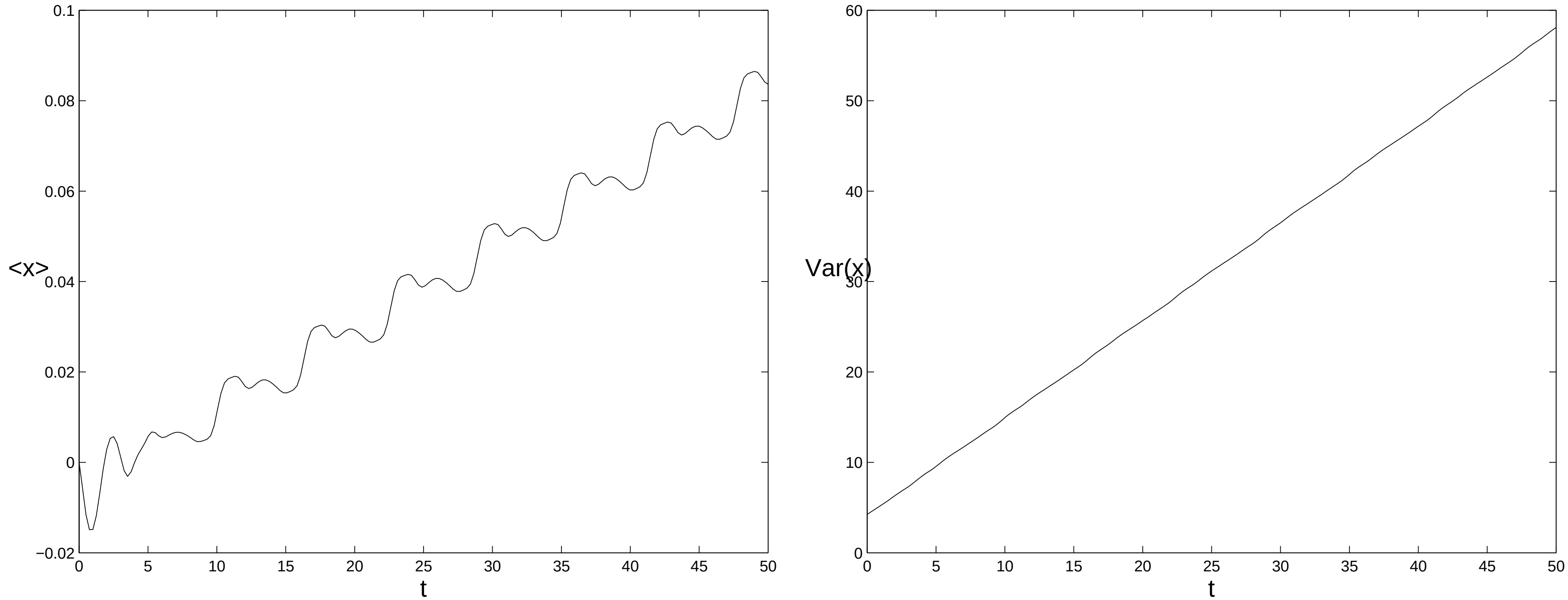
Note that here the drift is independent of time contrary to the previous case. The interplay between the two states can nevertheless produce a non zero asymptotic velocity.

Time evolution of the probability density $\rho_1(t,x) + \rho_2(t,x)$.



Displacement and variance



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In other words, $I(\nu_1, \nu_2, b_1, b_2) = \mathcal{O}(\vec{b}^3)$. This motor is in some sense less efficient that the previous one for small drifts.

A simple model with inertia (model III).

Another model of a particle interacting with a thermal bath is given by the Langevin equation

$$\begin{aligned} dx &= v\,dt \\ dv &= \big(-\gamma\, v + F(t,x)/m\big)\,dt + \sigma\, dW_t \end{aligned}$$

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where m is the mass of the particle, $\gamma > 0$ the friction coefficient, $F(t,x)$ the force, W_t the Brownian motion and $\sigma = \sqrt{\mathscr{D}}$ where $\mathscr{D}$ is the diffusion coefficient.

For the time evolution of the probability density $f(t, v, x)$ of the position and velocity of the particle one gets the so called Kramers equation

$$\partial_t f = -v\,\partial_x f + \partial_v\big[(\gamma v - F(t,x)/m)f\big] + \frac{\mathscr{D}}{2}\partial_v^2 f \ .$$

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We will assume as before that $F(t, x)$ is periodic of period T in time, L in space and with zero average in space and time. The average asymptotic velocity (more convenient for this model than the displacement, although trivially related) is defined by

$$I(\gamma, F) = \lim_{t\to\infty} \frac{1}{t} \int_0^t d\tau \iint v\, f(\tau, v, x)\, dv\, dx \ .$$

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Theorem 3

For $\gamma > 0$ and $F \in C^1_{per}(\mathbb{R}^2)$, $I(\gamma, F)$ is independent of the non negative initial distribution in $L^1((1+|v|)dx\,dv) \cap C^0_b(\mathbb{R}^2)$. The set of $F \in C^1_{per}(\mathbb{R}^2)$ with space average and time average equal to zero where $I(\gamma, F) \neq 0$ is open and dense.

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As in model (I), $I(\gamma, 0) = DI(\gamma, 0) = 0$ but $D^2 I(\gamma, 0) \neq 0$.

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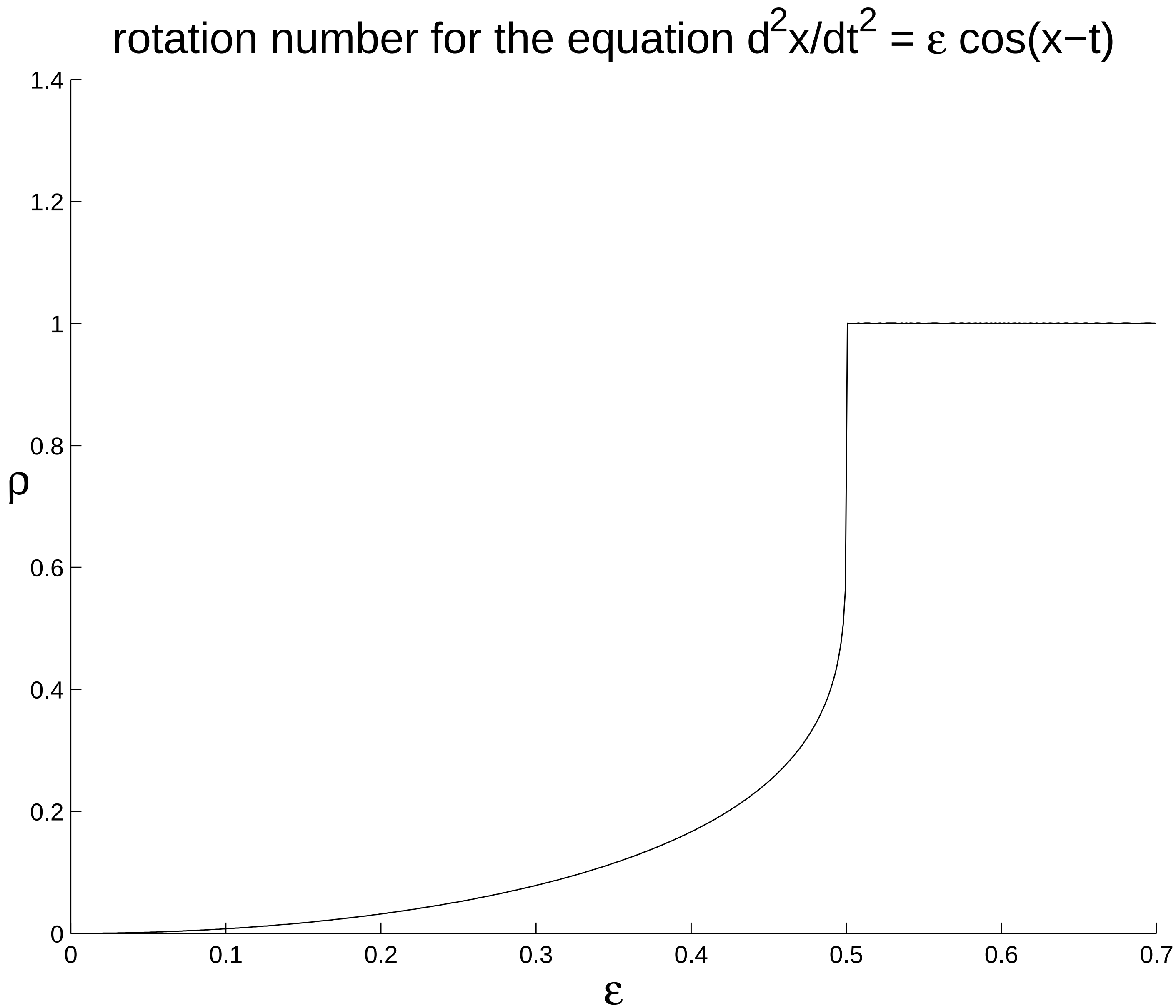

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\partial_t f_1 = &\ \tfrac{1}{2}\partial_v^2 f_1 - v\partial_x f_1 + \partial_v\big[(\gamma v - F_1(x))f_1\big] - \nu_1 f_1 + \nu_2 f_2 \\
\partial_t f_2 = &\ \tfrac{1}{2}\partial_v^2 f_2 - v\partial_x f_2 + \partial_v\big[(\gamma v - F_2(x))f_2\big] + \nu_1 f_1 - \nu_2 f_2 \ .
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In this equation, F_1 and F_2 are two periodic functions representing the different interaction forces between the two states of the particle and the substrate. The positive constants ν_1 and ν_2 are the transition rates between the two states. The non negative functions f_1 and f_2 are the probability densities of being in state one and two respectively. The total probability density of the particle is the function $f_1 + f_2$ which is normalised to one.

The asymptotic average velocity per unit time for this model is given by

$$I(\gamma, F_1, F_2, \nu_1, \nu_2) = \lim_{t \to \infty} \frac{1}{t} \int_0^t ds \iint v \left(f_1(s, v, x) + f_2(s, v, x) \right) dv dx,$$

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Theorem 4

For $\gamma > 0$, $\nu_1 > 0$ and $\nu_2 > 0$, and for any F_1 and F_2 in $C^1_{per}(\mathbb{R})$ $I(\gamma, F_1, F_2, \nu_1, \nu_2)$ is independent of the non negative initial distributions $f_1(0,v,x)$ and $f_2(0,v,x)$ in $L^1((1+|v|)dx\, dv) \cap C^0_b(\mathbb{R}^2)$. The set of F_1 and F_2 in $C^1_{per}(\mathbb{R})$ with space average equal to zero where $I(\gamma, F_1, F_2, \nu_1, \nu_2) \neq 0$ is open and dense.

In this model, we have also as in model (II) $I(\gamma, 0, 0, \nu_1, \nu_2) = DI(\gamma, 0, 0, \nu_1, \nu_2) = D^2 I(\gamma, 0, 0, \nu_1, \nu_2) = 0$, but $D^3 I(\gamma, 0, 0, \nu_1, \nu_2) \neq 0$.