Optimal Fluctuation Method

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Lecture 2

Part A. OFM for jump processes
Part B. OFM for (non-Markov) Gaussian processes

Part A: OFM for jump processes

Example: Extinction of established populations

A1. Extinction of a single well-mixed population due to “demographic noise”

A2. Extinction in two-population systems

Part 2A is mostly based on the topical review paper

M. Assaf and BM, J. Phys. A: Math. Theor. **50**, 263001 (2017)

Dodo. Extinct since the 17th century

Passenger pigeon. Extinct since the beginning of the 20th century

Extinction of an isolated population after maintaining a thriving long-lived state is a dramatic phenomenon. It ultimately occurs, even in the absence of detrimental environmental variations, because of a large fluctuation: an unusual chain of random events when population losses dominate over gains

Tasmanian wolf. Extinct since the 20th century

Consider a simple model of population extinction due to intrinsic (demographic) noise:

A single population of $n(t)$ individuals who multiply and die, as described by a Markov jump process

Single population

Example: SIS model (first appeared as a simple model of epidemic)

Nasell 1996,1999; Andersson and Djechiche 1998, Ovaskainen 2001, …

Birth and death rates
(or infection and recovery rates)

$$\lambda(n) = \lambda_0 n(K-n), \quad \mu(n) = \mu_0 n$$

Continuum deterministic rate equation

$$dn/dt = \lambda(n) - \mu(n), \quad \text{or}$$

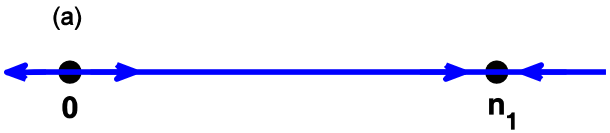
$$\frac{dq(t)}{dt} = \mu_0 q(R_0 - 1 - R_0 q), \qquad q = n/K, \;\; R_0 = \lambda_0 K/\mu_0$$

reproduction factor

$$R_0 > 1: \quad q = 0 \qquad \text{unstable fixed point}$$

$$q_1 = 1 - \frac{1}{R_0} \text{ stable fixed point, } \; t_r = \frac{1}{\mu_0(R_0 - 1)}$$

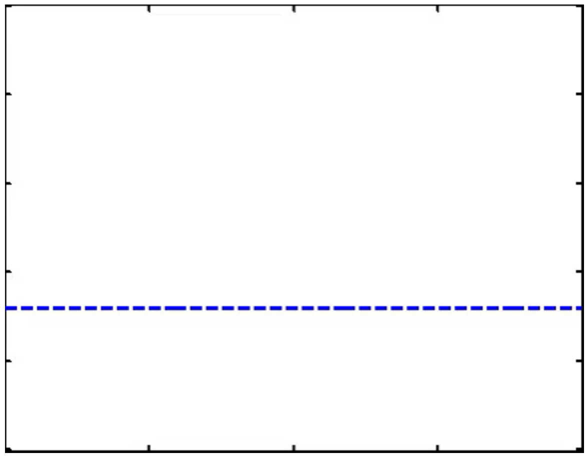
relaxation time



$$n_1 = K(1 - 1/R_0) >> 1$$

Discreteness of individuals and stochastic character of birth-death processes make a big difference!

a Monte Carlo simulation of the SIS model



Population ultimately goes extinct:

A sudden *large fluctuation* brings it into *absorbing state* n=0

Interesting to predict:

- Mean time to extinction (MTE)
- Extinction time statistics
- Quasi-stationary probability distribution of population sizes

Master equation for the Markov jump process

$P_n(t)$: probability of observing n individuals at time t

$P_0(t)$: probability of population extinction at time t

$$
\begin{cases}
\dfrac{dP_n}{dt} = \underbrace{\lambda_o\left[(n-1)(K-n+1)P_{n-1} - n(K-n)P_n\right]}_{\text{birth}} + \underbrace{\mu_0\left[(n+1)P_{n+1} - nP_n\right]}_{\text{death}}, \quad n = 1,2,3,\ldots \\
\dfrac{dP_0}{dt} = \mu_0 P_1
\end{cases}
$$

Previously available analytical methods for the MTE:

- single-step processes: exact solution, then asymptotics. Inapplicable to non-single-step processes
- Fokker-Planck approximation (aka "diffusion approximation") to the master equation: leads to exponentially large errors in the MTE

At $t \gg t_r$ extinction of established population proceeds as exponential decay of a long-lived *quasi-stationary* distribution (QSD): the first excited eigenstate of the master equation

$$P_n(t) \cong \pi_n \exp(-t/\tau),$$
$$P_0(t) \cong 1-\exp(-t/\tau).$$

π_n: QSD

τ : MTE, very large at $K \gg 1$

π_n and τ are the lowest non-trivial eigenstate and inverse eigenvalue of linear eigenvalue problem

$$\lambda_o\left[(n-1)(K-n+1)\pi_{n-1} - n(K-n)\pi_n\right] + \mu_0\left[(n+1)\pi_{n+1} - n\pi_n\right] = -\frac{1}{\tau}\pi_n \ , \quad n = 1,2,3,\ldots$$

$$\frac{1}{\tau} = \mu_0 \pi_1$$

π_n can be found in the WKB approximation: one of the names of the OFM

Kubo, Dykman et al, Elgart and Kamenev, Assaf and M, Kessler and Shnerb,...

$$\lambda_o\left[(n-1)(K-n+1)\pi_{n-1}-n(K-n)\pi_n\right]+\mu_0\left[(n+1)\pi_{n+1}-n\pi_n\right]=-\frac{1}{\tau}\pi_n\ ,\quad n=1,2,3,\ldots$$

$$\frac{1}{\tau}=\mu_0\pi_1$$

The WKB ansatz

$$\pi_n=\exp[-KS(q)],\qquad q=n/K,\quad K>>1$$

$$S(q)=S_0(q)+\frac{1}{K}S_1(q)+\frac{1}{K^2}S_2(q)+\ldots$$

where, for n>>1, we treat S(q) as a smooth function

$$\pi_{n-1}=\exp[-KS(\tfrac{n-1}{K})]=\exp[-KS_0(q)+S_0'(q)+\ldots]$$

$$\pi_{n+1}=\exp[-KS(\tfrac{n+1}{K})]=\exp[-KS_0(q)-S_0'(q)+\ldots]$$

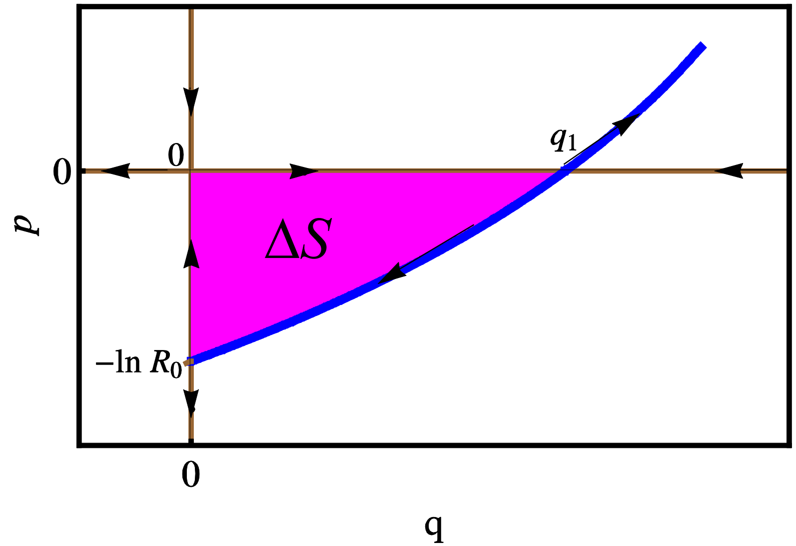
In the leading order in 1/K we obtain a time-independent Hamilton-Jacobi equation

$$H_0(q, \frac{dS_0}{dq}) \cong 0$$

with the Hamiltonian

$$H_0(q,p) = \mu_0 q\left[R_0(1-q)\left(e^p - 1\right) + e^{-p} - 1\right], \qquad p = \partial_q S$$

The optimal path to extinction is a zero-energy trajectory of effective mechanical system



Relaxation trajectory: p=0, deterministic rate equation

The optimal path to extinction – activation trajectory – is a heteroclinic trajectory connecting fixed points ($q=q_1$, $p=0$) and ($q=0$, $p=-\ln R_0$)
It does not coincide with the time-reversed relaxation trajectory!

$$p(q) = \ln\left[\frac{1}{R_0(1-q)}\right], \qquad \Delta S = \int_{q_1}^{0} p(q)\, dq = \ln R_0 + \frac{1}{R_0} - 1$$

extinction rate function

Mean time to extinction is, up to a pre-factor,

$$\tau \sim \exp(K\Delta S) = \exp\left[K\left(\ln R_0 + \frac{1}{R_0} - 1\right)\right], \qquad K\Delta S >> 1$$

exponentially long in K

Close to the transcritical bifurcation, $\delta = R_0 - 1 << 1$, the result is universal for a whole class of models:

$$\tau \sim \exp\left(\frac{1}{2}K\delta^2\right), \qquad K\delta^2 >> 1$$

Pre-exponential factor can be also calculated, by matching the subleading-order WKB solution with a recursive solution of the master equation for small n

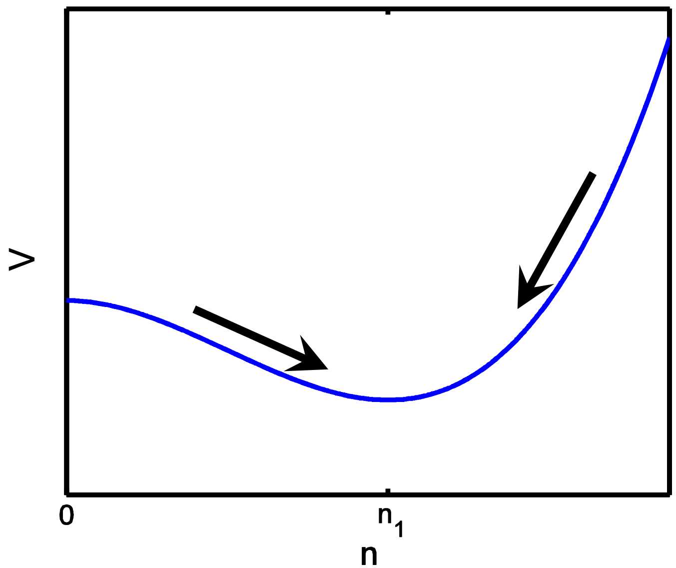
M. Assaf and BM 2007,2010, Kessler and Shnerb 2007

Now let's go back to the deterministic rate equation and rewrite it as

$$\frac{dq}{dt} = -\frac{d}{dq}V(q),$$

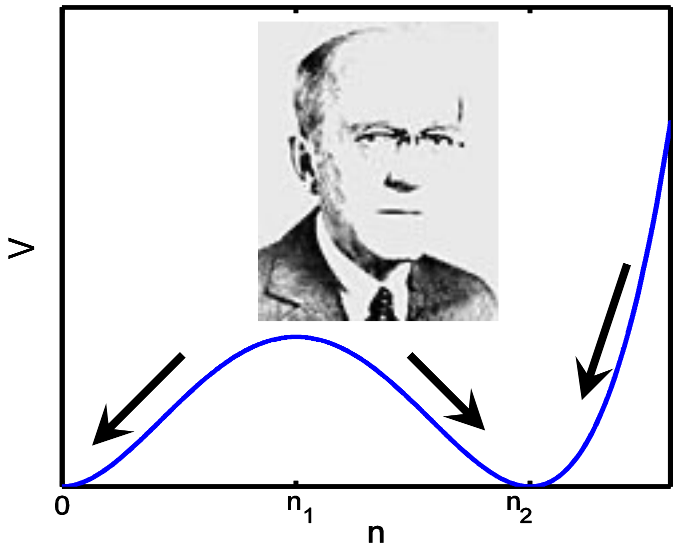
overdamped "particle motion in a potential"

SIS model: no Allee effect



monostability: $q=q_1$

Allee effect

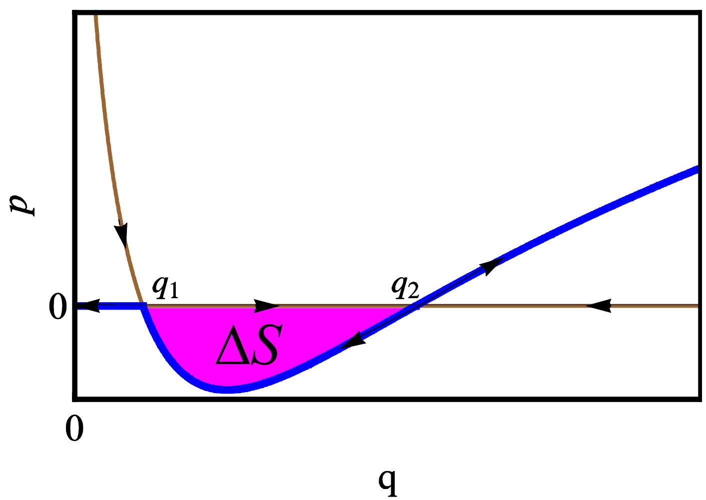


bistability: $q=0$ and $q=q_2$

Warder C. Allee (1885-1955)

Mean time to extinction with account of Allee effect

Using WKB approximation



A different heteroclinic trajectory in q,p plane

Mean time to extinction is, up to pre-exponent,

$$\tau \sim \exp(K\Delta S)$$

Elgart and Kamenev 2006

Close to the saddle-node bifurcation, $\delta \ll 1$, the result is universal for a whole class of models with strong Allee effect:

$$\tau \sim \exp\left(\alpha K\delta^3\right), \quad \alpha = O(1), \qquad K\delta^3 >> 1$$

Prefactor has been also determined

BM and P.V. Sasorov 2009, C. Escudero and A. Kamenev 2009, M. Assaf and BM 2010

Two-population systems: extinction of epidemics

Example: SI (Susceptible-Infected) model with population turnover

Captures essence of most common childhood diseases that confer long-lasting immunity: measles, mumps and rubella

Event	Type of transition	Rate
Infection	$S \to S-1,\ I \to I+1$	$(\beta/N)SI$
Renewal of susceptible	$S \to S+1$	μN
Removal of infected	$I \to I-1$	ΓI
Removal of susceptible	$S \to S-1$	μS

Deterministic rate equations

$$\frac{dS}{dt} = \mu N - \mu S - \frac{\beta}{N} SI,$$

$$\frac{dI}{dt} = \frac{\beta}{N} SI - \Gamma I.$$

$$\frac{dS}{dt} = \mu N - \mu S - \frac{\beta}{N} SI,$$
$$\frac{dI}{dt} = \frac{\beta}{N} SI - \Gamma I.$$

β < Γ: only infection-free steady state: attracting fixed point *S=N, I=0*

β > Γ: point S=N, I=0 is repelling. Now attracting *endemic* point appears:

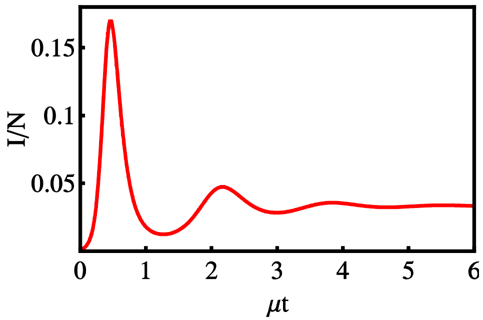
$$\bar{S} = \frac{\Gamma}{\beta} N, \qquad \bar{I} = \left(\frac{1}{\Gamma} - \frac{1}{\beta}\right) N$$

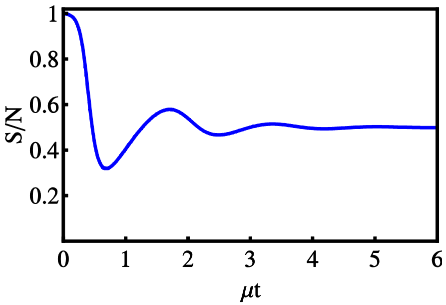
N>>1

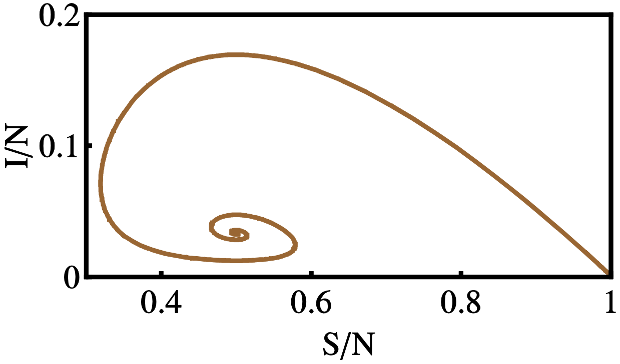
$$\mu < 4(\beta - \Gamma)(\Gamma / \beta)^2$$

Endemic fixed point is a stable focus

epidemic dynamics is oscillatory: multiple outbreaks of disease





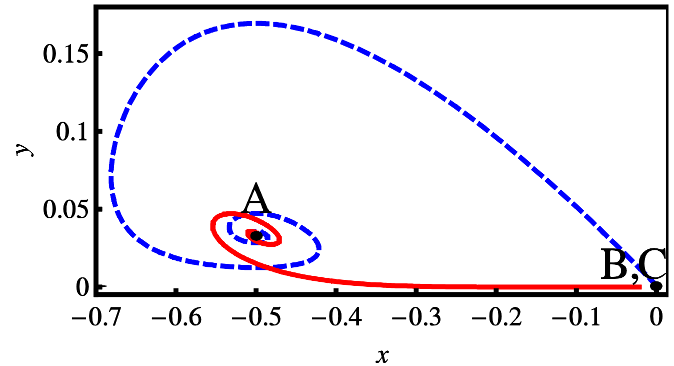


$$\mu > 4(\beta - \Gamma)(\Gamma / \beta)^2$$

Endemic fixed point is a stable node

Stochastic dynamics: $P_{nm}(t)$ is "leaking" into disease-free state.

OFM: The most likely disease extinction trajectory is a heteroclinic orbit in a 4-dimensional phase space: it exits from fixed point A and reaches the extinction hyperplane x=0 at fixed point B:



deterministic trajectory

optimal path to disease extinction, found numerically

$x=S/N$

$y=I/N$

$$A=[-\delta,(\delta/K)(1-\delta)^{-1},0,0]$$

$$B=[0,0,0,\ln(1-\delta)]$$

$$C=[0,0,0,0]$$

A. Kamenev and BM Phys. Rev. E **77**, 061107(2008)

Related problems

• Extinction in two-population systems occupying a fixed point: other epidemic models (M. Dykman et al. 2008, …), switching between active and dormant phenotypes (I. Lohmar and BM 2011), minimizing extinction risk by migration between sites (M. Khasin et al. 2012), competition between two species (A. Gabel et al. 2013),…

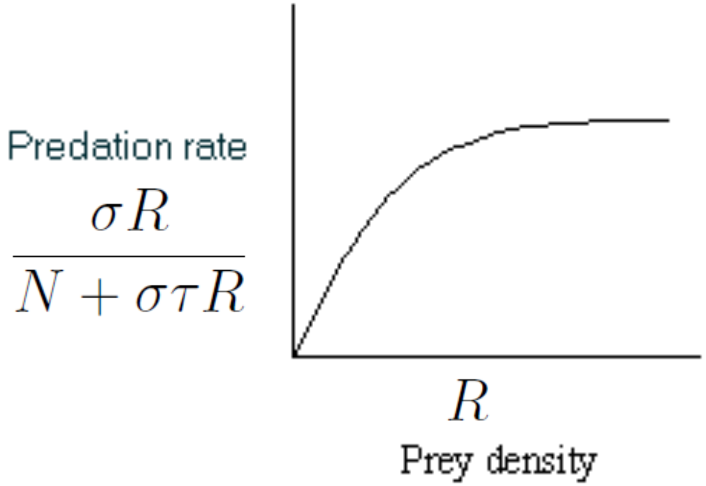
• Optimization of selective vaccination protocols
M. Khasin et al. 2010, …

Extinction of oscillating populations, or extinction from a limit cycle

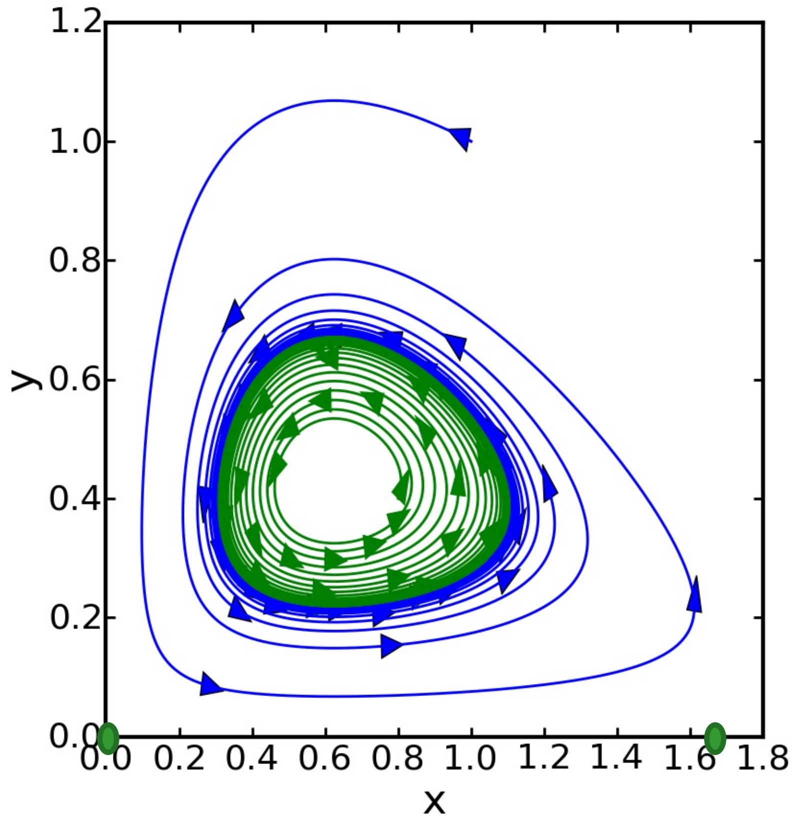
Example: predator-prey model with prey competition and predator satiation (Rosenzweig and MacArthur 1963)

$$\dot{R} = aR - \frac{1}{2N}R^2 - \frac{\sigma R F}{N + \sigma\tau R}$$

$$\dot{F} = -F + \frac{\sigma R F}{N + \sigma\tau R}$$



$\sigma > \sigma^*$ Limit cycle

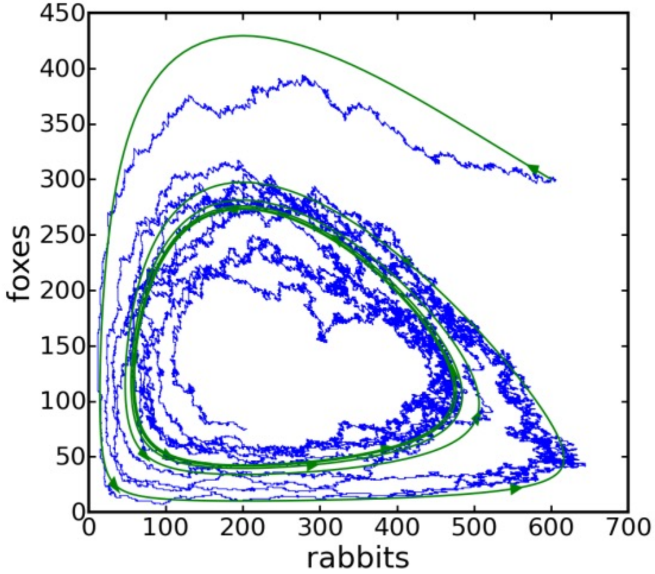


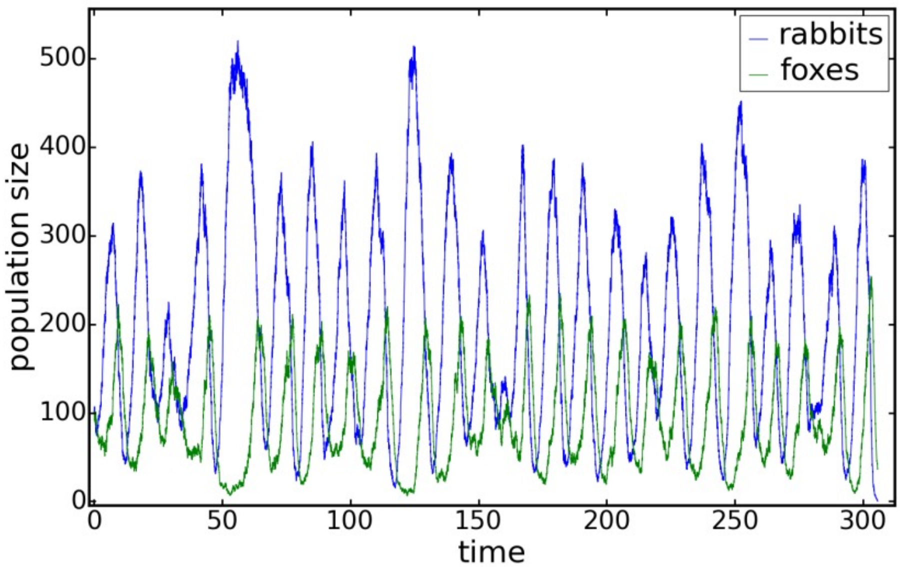
x=R/N
y=F/N

Stochastic version of the Rosenzweig and MacArthur model

N.R. Smith and BM, Phys. Rev. E **93**, 032109 (2016)

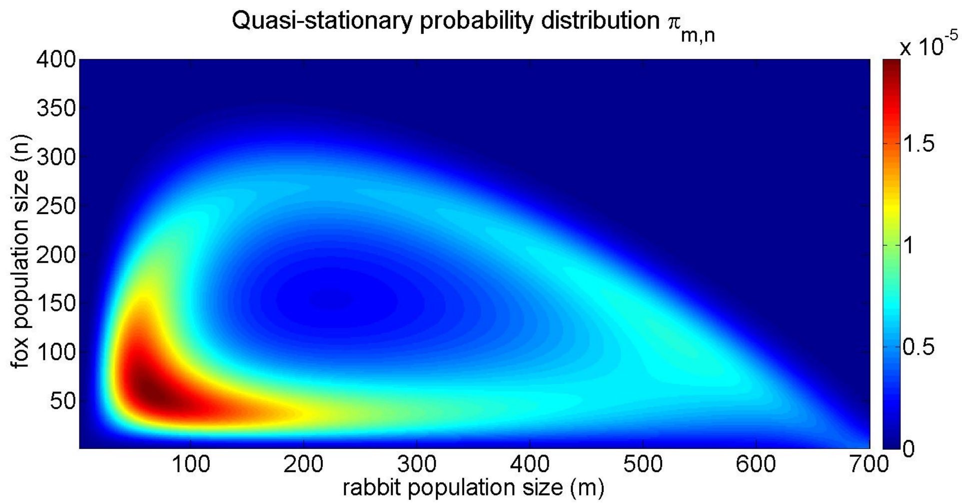
$$
\begin{aligned}
R &\to 2R \\
2R &\to R \\
F + R &\to 2F \\
F &\to 0
\end{aligned}
$$





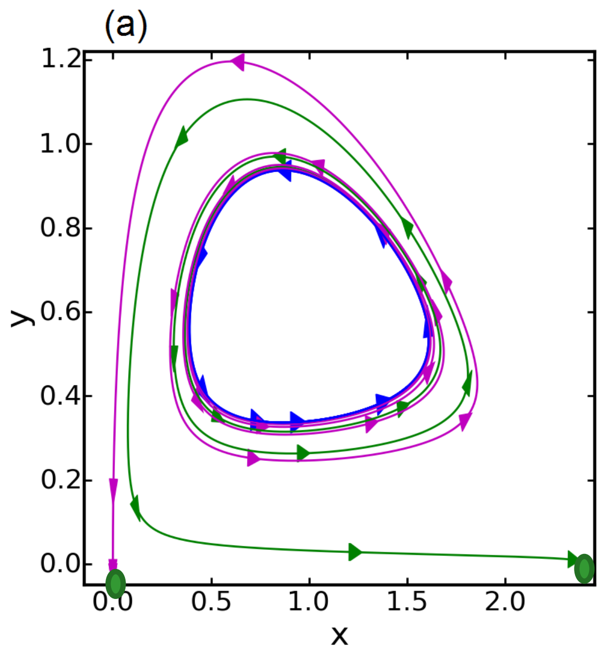
Master equation for the stochastic RMA model

$$\begin{aligned}
\dot{P}_{m,n} &= \underbrace{a\left[(m-1)\,P_{m-1,n} - mP_{m,n}\right]}_{\text{rabbit birth}} + \\
&+ \underbrace{\left[\frac{\sigma\,(m+1)\,(n-1)}{N+\sigma\tau\,(m+1)}P_{m+1,n-1} - \frac{\sigma mn}{N+\sigma\tau m}P_{m,n}\right]}_{\text{predation}} + \\
&+ \underbrace{(n+1)\,P_{m,n+1} - nP_{m,n}}_{\text{fox death}} + \\
&+ \underbrace{\frac{1}{2N}\left[(m+1)\,mP_{m+1,n} - m\,(m-1)\,P_{m,n}\right]}_{\text{rabbit death due to competition}}
\end{aligned}$$



OFM Hamiltonian

$$H = ax\left(e^{p_x}-1\right)+\frac{\sigma x y}{1+\sigma\tau x}\left(e^{p_y-p_x}-1\right)+ y\left(e^{-p_y}-1\right)+\frac{1}{2}x^2\left(e^{-p_x}-1\right)=0$$



optimal paths to extinction

- extinction rates/times
- relative probabilities of two extinction routes
- change of these at the Hopf bifurcation of the birth of the limit cycle

Results of part A

- OFM provides a systematic method of evaluating the mean time to extinction of long-lived populations.
- More generally, OFM provides a valuable insight into large deviations of Markov jump processes.

Part B: OFM for non-Markov Gaussian processes

Example: Thermally activated particle motion in disordered Gaussian potentials

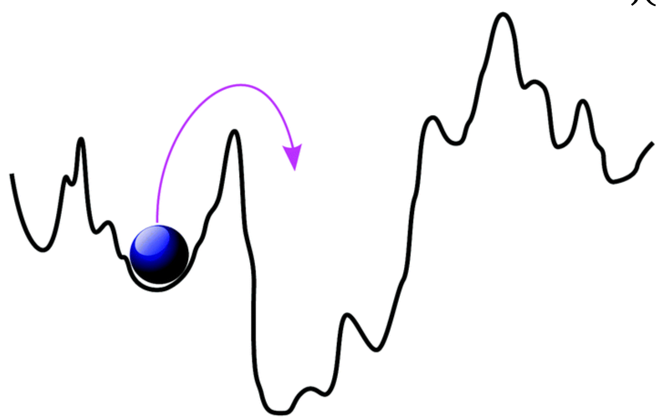
Part 2B is based on papers

BM, Phys. Rev. E **105**, 034106 (2022); **107**, 039902 (2023);
A.Valov, N. Levi and BM, arXiv:2405.09850.

Simple transport model: overdamped particle in a short-correlated quenched disorder potential $V(x)$ in presence of thermal noise

$$\frac{dx}{dt} = -\frac{dV(x)}{dx} + \sqrt{2D}\,\xi(t)$$

$V(x)$: *disorder potential*
D: *the particle diffusion coefficient in the absence of disorder*
$\xi(t)$: delta-correlated Gaussian noise with zero mean and $< \xi(t)\, \xi(t') > = \delta\,(t-t')$



At low temperature, $D \to 0$, the particle rapidly settles down in a local potential minimum, but ultimately escapes by overcoming a potential barrier $\Delta V = V_{max} - V_{min}$

The mean escape time over one such potential barrier is $T \sim \exp(\Delta V / D)$ (Kramers 1940). Here the averaging is performed over the thermal noise.

Activated escape of particles in quenched disorder potentials is an important paradigm in many applications:

- diffusive transport of electrons, holes, and excitons in disordered metals or semiconductors
- viscous flow of supercooled liquids and glassy matrices
- DNA macromolecules in living systems
- Colloidal systems in quenched random potentials, created by laser light, have recently become experimentally available

P. G. De Gennes, J. Stat. Phys. **12**, 463 (1975)
H. Bässler, Phys. Rev. Lett. **58**, 767 (1987)
R. Zwanzig, Proc. Natl. Acad. Sci. USA **85**, 2029 (1988)
A. V. Lopatin and V. M. Vinokur, Phys. Rev. Lett. **86**, 1817 (2001)
I. Goychuk, V.O. Kharchenko, and R. Metzler, Phys. Rev E **96**, 052134 (2017)
M. Wilkinson, M. Pradas, and G. Kling, J. Stat. Phys. **182**, 54 (2021)

Our main goal: evaluate the mean escape time $\langle T \rangle$, where the additional averaging is performed **over realizations of the disorder potential**

Let $P(\Delta V)$ be the distribution of the potential barriers

Key observation: at $D \to 0$, $\langle T \rangle$ is dominated by the $\Delta V \to \infty$ tail of $P(\Delta V)$.
This tail is expected to behave as $P(\Delta V \to \infty) \sim \exp[-s(\Delta V)]$
with some a priori unknown $s(\Delta V)$

$$\langle T \rangle \sim \int d\Delta V \exp\left(\frac{\Delta V}{D} - s(\Delta V)\right)$$

$D \to 0$: the integral can be evaluated by the Laplace's method:

$$\langle T \rangle \sim \exp\left(\frac{\Delta V_s}{D} - s(\Delta V_s)\right)$$

The saddle point ΔV_s is determined from the equation $D\frac{ds(\Delta Vs)}{d\Delta V_s} = 1$

We need to determine $s(\Delta V)$

Suppose that the potential $V(x)$ is statistically homogeneous and normally distributed with zero mean (no systematic bias) and autocovariance

$$\langle V(x) V(x') \rangle = \kappa(x-x'), \text{ where } \quad \kappa(-z) = \kappa(z)$$

The inverse kernel $K(x-x')$ is defined by

$$\int_{-\infty}^{\infty} dx'' \, K(x - x'')\kappa(x' - x'') = \delta(x - x')$$

The knowledge of $K(z)$ enables us to write down the statistical weight of a given realization of a normally distributed random field $V(x)$.

Up to normalization, the statistical weight is ~ exp(-S[V(x)]), with nonlocal action functional

$$S[V(x)] = \frac{1}{2}\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dx' K(x-x')V(x)V(x')$$

Key observation: The distribution tail $P(\Delta V \to \infty)$, which corresponds to atypically large ΔV, is dominated by the *optimal* (that is, most likely) configuration of the potential $V(x)$ conditioned on this ΔV .

Recipe: minimize the nonlocal action functional $S[V(x)]$ over realizations of $V(x)$ subject to constraint on ΔV. The latter can be accounted for via a Lagrange multiplier λ.

We can place the adjacent minimum and maximum of $V(x)$ at $x=-L$ and $x=L$

$$V(x=L) - V(x=-L) = \Delta V > 0,$$

$$\frac{dV}{dx}(x=-L) = 0, \qquad \frac{dV}{dx}(x=L) = 0,$$

$$\frac{d^2V}{dx^2}(x=-L) > 0, \qquad \frac{d^2V}{dx^2}(x=-L) < 0,$$

$$\frac{dV}{dx}(|x| < L) > 0$$ differential inequality

If necessary, minimize the action S over all possible values of L

Introducing a Lagrange multiplier λ, we can minimize the functional

$$S_\lambda[V(x)] = \frac{1}{2}\int_{-\infty}^{\infty} dx\,\{\int_{-\infty}^{\infty} dx' K(x-x')V(x)V(x')$$
$$-\lambda\, V(x)[\delta(x-L)-\delta(x+L)]\,\}.$$

The linear variation must vanish, leading to the linear integral equation

$$\int_{-\infty}^{\infty} dx'\, K(x-x')V(x') = \frac{\lambda}{2}[\delta(x-L)-\delta(x+L)]\,.$$

Comparing it with the definition of the inverse kernel $K(z)$,

$$\int_{-\infty}^{\infty} dx''\, K(x-x'')\kappa(x'-x'') = \delta(x-x')$$

we can easily guess the solution:

$$V(x) = \frac{\lambda}{2}[\kappa(x-L)-\kappa(x+L)].$$

Solution for given distance L between max and min:

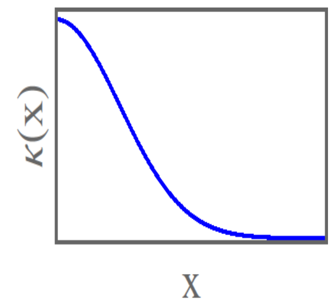
$$V(x) = \frac{\lambda}{2}[\kappa(x - L) - \kappa(x + L)].$$

Now we demand that $x = L$ be a maximum:

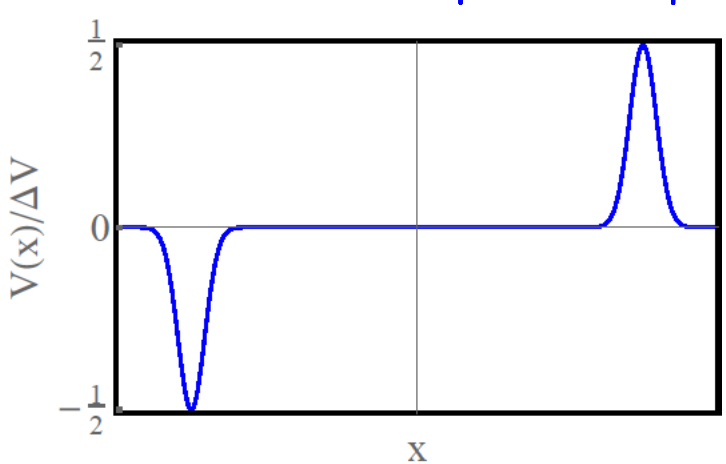
$$\frac{d\kappa(x)}{dx}(x = 0) - \frac{d\kappa(x)}{dx}(x = 2L) = 0. \qquad (1)$$

For smooth $\kappa(x)$ the first term vanishes. Now everything depends on whether $\kappa(x)$ is monotone decreasing or not.

1. $\kappa(x)$ is monotone decreasing



To satisfy Eq. (1) we must choose $L = \infty$: the optimal configuration of $V(x)$ consists of two independent "pulses" of the potential.



The pulse shape coincides with that of $\kappa(x)$

The action

$$S[V(x)] = \frac{1}{2}\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dx' K(x-x')V(x)V(x') = \frac{\Delta V^2}{4\,\kappa(0)}$$

This Gaussian tail depends only on the disorder variance; independent of $\kappa(x)$.

$$\Longrightarrow \quad < T > \sim \exp\left(\frac{\kappa(0)}{D^2}\right), \qquad D \to 0$$

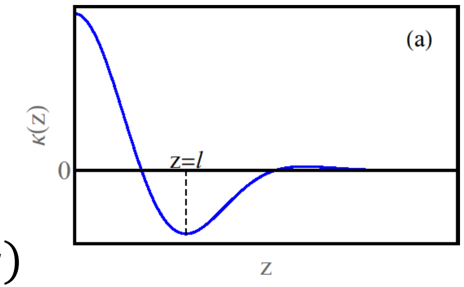
Agrees with De Gennes 1975, Zwanzig 1988, ...

who predicted a giant suppression of activated diffusion by disorder

$$V(x) = \frac{\lambda}{2}[\kappa(x-L) - \kappa(x+L)].$$

$$\frac{d\kappa(x)}{dx}(x=0) - \frac{d\kappa(x)}{dx}(x=2L) = 0.$$

2. $\kappa(x)$ is non-monotonic



Let $x = l > 0$ be the first minimum point of $\kappa(x)$

As a result, L= $\frac{l}{2}$

The optimal configuration: $V(x) = \frac{\Delta V}{2}\frac{\kappa\left(x-\frac{l}{2}\right) - \kappa\left(x+\frac{l}{2}\right)}{\kappa(0)-\kappa(l)}$

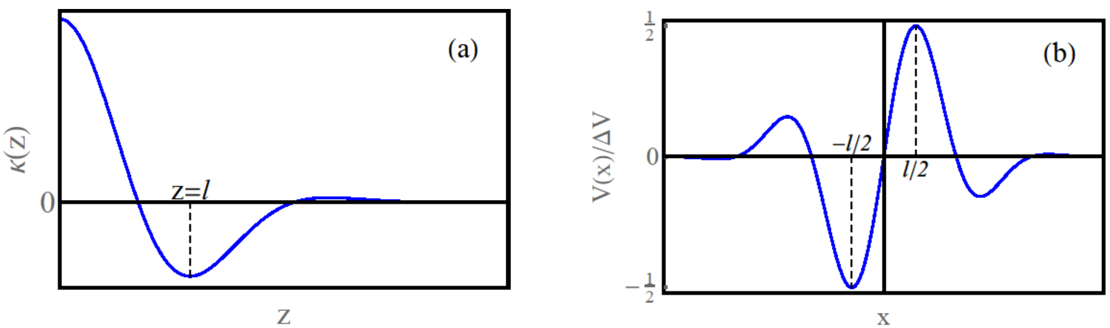
$$s(\Delta V) = \frac{\Delta V^2}{4\,[\kappa(0) - \kappa(l)]}, \qquad < T > \sim \exp\left(\frac{\kappa(0) - \kappa(l)}{D^2}\right)$$

A more interesting result: it depends on the autocovariance!

Two subcases of non-monotonic correlations

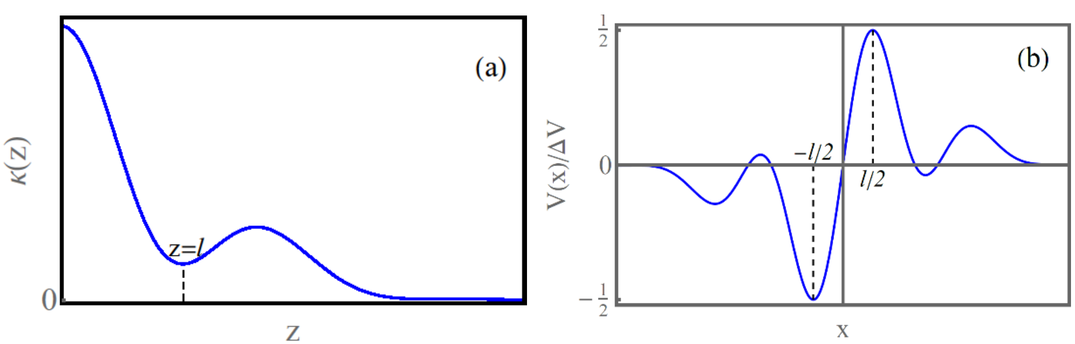
$$s(\Delta V) = \frac{\Delta V^2}{4\,[\kappa(0) - \kappa(l)]}, \qquad < T > \sim \exp\left(\frac{\kappa(0) - \kappa(l)}{D^2}\right)$$

A. Negative correlations are present: $\kappa(l) < 0$



$\kappa(l) < 0$: Activated escape is exponentially suppressed

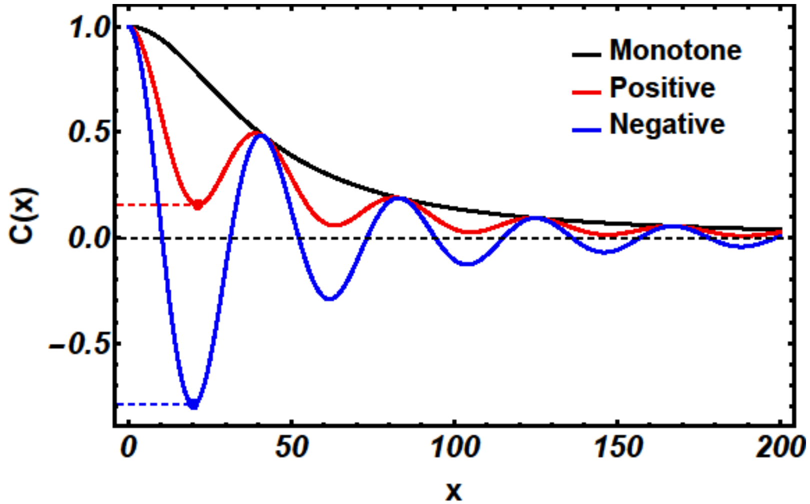
B. Correlations are everywhere positive: $\kappa(l) > 0$



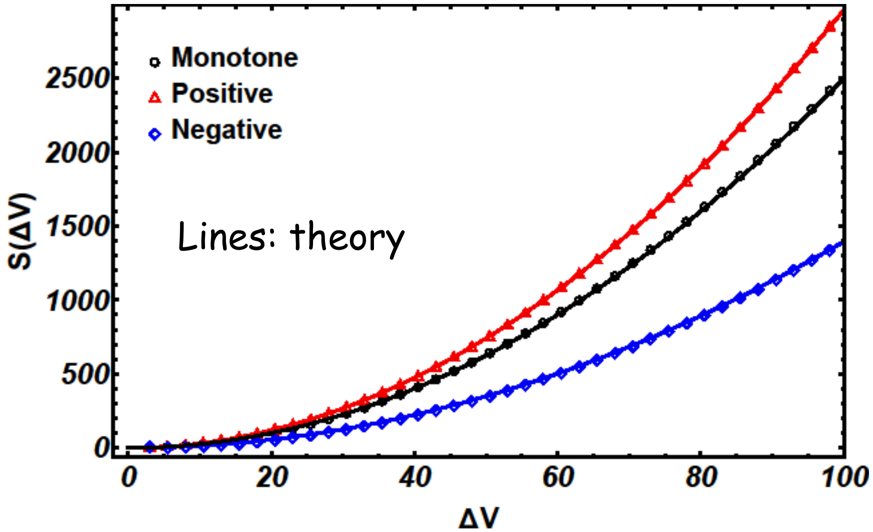
$\kappa(l) > 0$: Activated escape is exponentially enhanced

Large-deviation Monte-Carlo simulations

We used correlated random discretized potential sampling based on the Wang-Landau algorithm, the circulant embedding method and discrete Fourier transform, please ask Alexander Valov for details. This allowed us to measure probability densities smaller than 10^{-1200}



Measured action $S(\Delta V) = -\ln P(\Delta V)$

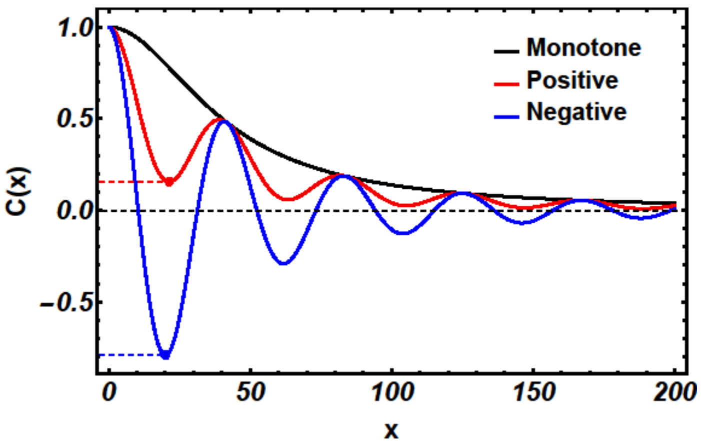


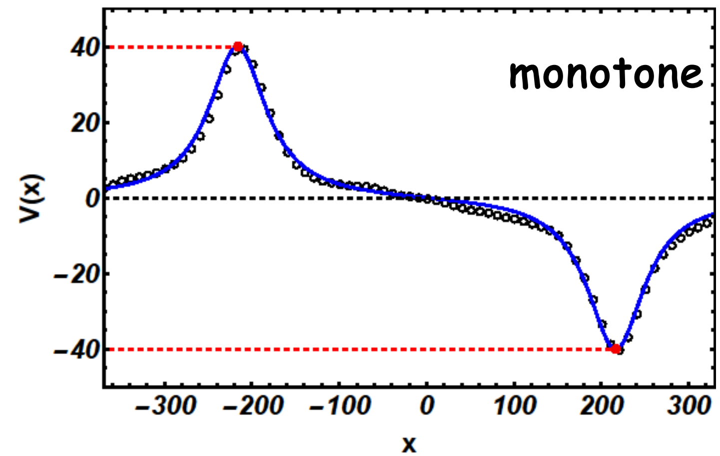
A.Valov, N. Levi and BM, arXiv:2405.09850.

Large-deviation Monte-Carlo simulations

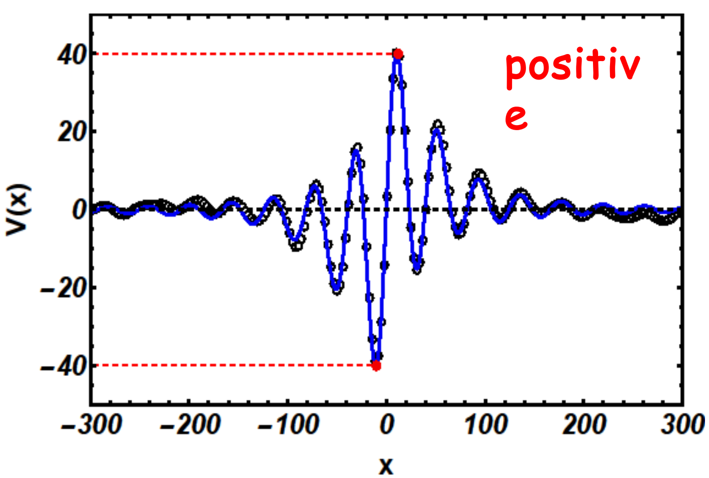
Optimal realizations of the potential V(x)

Lines: theory, symbols: simulations

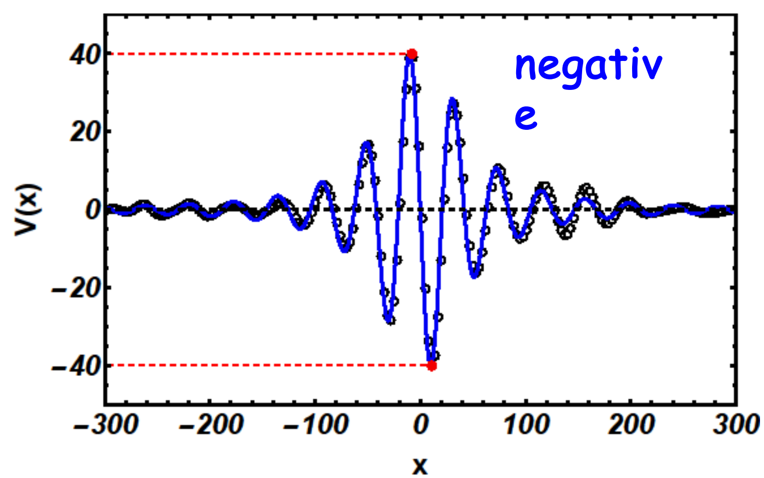




fitted L



no fitting parameters

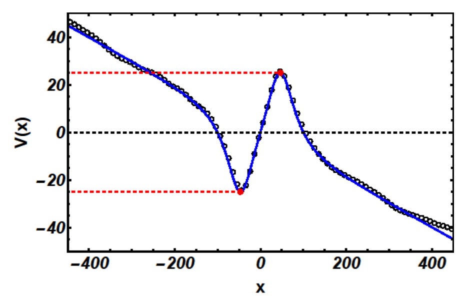


Results of part B

- Non-monotonic correlations of disorder in 1d strongly (exponentially) affect the mean time to activated escape of overdamped particles.
- Quantitative modeling of particle transport in disordered media at low temperatures may require a more detailed knowledge of the autocorrelation properties of the disorder than it was believed previously.
- Optimal fluctuation method provides a valuable insight into large deviations of non-Markovian Gaussian processes.

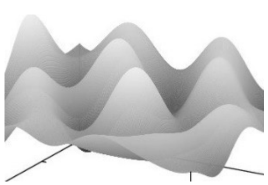
Extensions

- Bias of potential: $V(x) = V_{random}(x) + Fx$
  Done.
  A.Valov, N. Levi and BM, arXiv:2405.09850



Line: theory
symbols: simulations

- Extend to higher dimensions? Activated escape over a saddle, rather than over a maximum. Not done yet.



Additional applications of OFM: a partial and subjective list

Markov processes:

1. Brownian acceleration: BM, Geometrical optics of first-passage functionals of random acceleration, Phys. Rev. E **107**, 064122 (2023).

2. Non-Markov Gaussian processes:

a. Anomalous scaling of dynamical large deviations of stationary Gaussian processes. BM, Phys. Rev. E **100**, 042135 (2019).
b. Geometrical optics of large deviations of fractional Brownian motion, BM and G. Oshanin, Phys. Rev. E **105**, 064137 (2022).
c. First-passage area distribution and optimal fluctuations of fractional Brownian motion. A. K. Hartmann and B. Meerson, Phys. Rev. E **109**, 014146 (2024).
d. Fractional Brownian motion in confining potentials: non-equilibrium distribution tails and optimal fluctuations. BM and P. Sasorov, arXiv:2407.0861.

Time-dependent random fields:

3. Large deviations in turbulence and turbulent transport (the Burgers equation, the passive scalar equation): since late 90-ies.

4. MFT of lattice gases: almost a hundred papers by now. Stationary and nonstationary settings, exact integrability of selected models by the Inverse Scattering Method (ISM), extensions to long-range interactions, active fluids,,…

5. Extinction of spatially distributed populations.

6. Large deviations of one-point interface height in the KPZ equation and other surface growth models, exact integrability by the ISM.