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The Effect of Gaussian White Noise on Dynamical Systems: Diffusion Exit from a Domain

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Introduction: A Brownian particle in a potential

Small random perturbations

Gradient dynamics (ODE)

$$\dot{x}_t^{\text{det}} = -\nabla V(x_t^{\text{det}})$$

Random perturbation by Gaussian white noise (SDE)

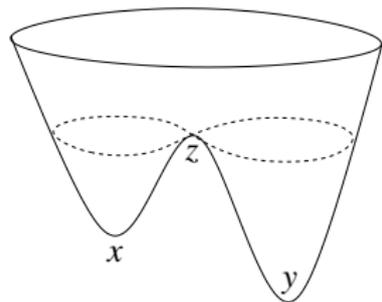
$$dx_t^\varepsilon(\omega) = -\nabla V(x_t^\varepsilon(\omega)) dt + \sqrt{2\varepsilon} dB_t(\omega)$$

Equivalent notation

$$\dot{x}_t^\varepsilon(\omega) = -\nabla V(x_t^\varepsilon(\omega)) + \sqrt{2\varepsilon}\xi_t(\omega)$$

with

- ▷ $V : \mathbb{R}^d \rightarrow \mathbb{R}$: confining potential, growth condition at infinity
- ▷ $\{B_t(\omega)\}_{t \geq 0}$: d -dimensional Brownian motion
- ▷ $\{\xi_t(\omega)\}_{t \geq 0}$: Gaussian white noise, $\langle \xi_t \rangle = 0$, $\langle \xi_t \xi_s \rangle = \delta(t - s)$



Fokker–Planck equation

Stochastic differential equation (SDE) of gradient type

$$dx_t^\varepsilon(\omega) = -\nabla V(x_t^\varepsilon(\omega)) dt + \sqrt{2\varepsilon} dB_t(\omega)$$

Kolmogorov's forward or Fokker–Planck equation

- ▷ Solution $\{x_t^\varepsilon(\omega)\}_t$ is a (time-homogenous) Markov process
- ▷ Densities $(x, t) \mapsto p(x, t|y, s)$ of the transition probabilities satisfy

$$\frac{\partial}{\partial t} p = \mathcal{L}_\varepsilon p = \nabla \cdot [\nabla V(x)p] + \varepsilon \Delta p$$

- ▷ If $\{x_t^\varepsilon(\omega)\}_t$ admits an invariant density p_0 , then $\mathcal{L}_\varepsilon p_0 = 0$
- ▷ Easy to verify (for gradient systems)

$$p_0(x) = \frac{1}{Z_\varepsilon} e^{-V(x)/\varepsilon} \quad \text{with} \quad Z_\varepsilon = \int_{\mathbb{R}^d} e^{-V(x)/\varepsilon} dx$$

Equilibrium distribution

- ▷ **Invariant measure** or **equilibrium distribution**

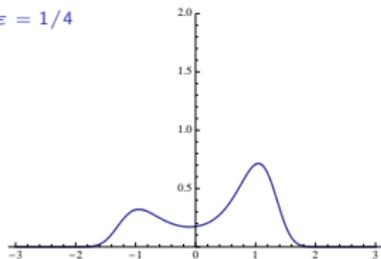
$$\mu_\varepsilon(dx) = \frac{1}{Z_\varepsilon} e^{-V(x)/\varepsilon} dx$$

- ▷ System is **reversible** w.r.t. μ_ε (detailed balance)

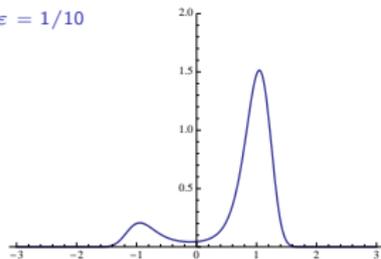
$$p(y, t|x, 0) e^{-V(x)/\varepsilon} = p(x, t|y, 0) e^{-V(y)/\varepsilon}$$

- ▷ For small ε , invariant measure μ_ε concentrates in the minima of V

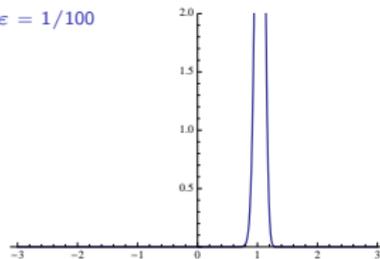
$\varepsilon = 1/4$



$\varepsilon = 1/10$



$\varepsilon = 1/100$



Timescales

Let V double-well potential as before, start in $x_0^\varepsilon = x_-^* = \text{left-hand well}$

How long does it take until x_t^ε is well described by its invariant distribution?

- ▶ For ε small, paths will stay in the left-hand well for a long time
- ▶ x_t^ε first approaches a Gaussian distribution, centered in x_-^* ,

$$T_{\text{relax}} = \frac{1}{V'''(x_-^*)} = \frac{1}{\text{curvature at the bottom of the well}} \quad (d=1)$$

- ▶ With overwhelming probability, paths will remain inside left-hand well, for all times significantly shorter than **Kramers' time**

$$T_{\text{Kramers}} = e^{H/\varepsilon}, \quad \text{where } H = V(z^*) - V(x_-^*) = \text{barrier height}$$

- ▶ Only for $t \gg T_{\text{Kramers}}$, the distribution of x_t^ε approaches p_0

The dynamics is thus very different on the different timescales

Diffusion exit from a domain

The more general picture: Diffusion exit from a domain

$$dx_t^\varepsilon = b(x_t^\varepsilon) dt + \sqrt{2\varepsilon}g(x_t^\varepsilon) dW_t, \quad x_0 \in \mathbb{R}^d$$

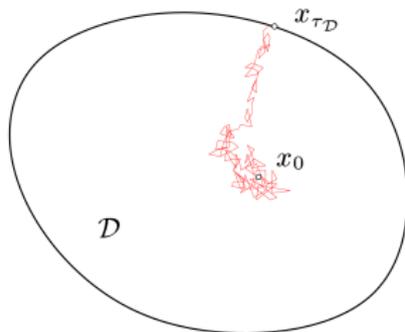
General case: b not necessarily derived from a potential

Consider bounded domain $\mathcal{D} \ni x_0$ (with smooth boundary)

- ▷ First-exit time: $\tau = \tau_{\mathcal{D}}^\varepsilon = \inf\{t > 0: x_t^\varepsilon \notin \mathcal{D}\}$
- ▷ First-exit location: $x_\tau^\varepsilon \in \partial\mathcal{D}$

Questions

- ▷ Does x_t^ε leave \mathcal{D} ?
- ▷ If so: When and where?
- ▷ Expected time of first exit?
- ▷ Concentration of first-exit time and location?
- ▷ **Distribution of τ and x_τ^ε ?**



First case: Deterministic dynamics leaves \mathcal{D}

If x_t leaves \mathcal{D} in finite time, so will x_t^ε . Show that deviation $x_t^\varepsilon - x_t$ is small:

Assume b Lipschitz continuous and $g = \text{Id}$

$$\|x_t^\varepsilon - x_t\| \leq L \int_0^t \|x_s^\varepsilon - x_s\| ds + \sqrt{2\varepsilon} \|W_t\|$$

By Gronwall's lemma

$$\sup_{0 \leq s \leq t} \|x_s^\varepsilon - x_s\| \leq \sqrt{2\varepsilon} \sup_{0 \leq s \leq t} \|W_s\| e^{Lt}$$

▷ $d = 1$: Use André's reflection principle

$$\mathbb{P} \left\{ \sup_{0 \leq s \leq t} |W_s| \geq r \right\} \leq 2 \mathbb{P} \left\{ \sup_{0 \leq s \leq t} W_s \geq r \right\} \leq 4 \mathbb{P} \{ W_t \geq r \} \leq 2 e^{-r^2/2t}$$

▷ $d > 1$: Reduce to $d = 1$ using independence

▷ **General case**: Use large-deviation principle

Second case: Deterministic dynamics does not leave \mathcal{D}

Assume \mathcal{D} **positively invariant** under deterministic flow: Study **noise-induced** exit

$$dx_t^\varepsilon = b(x_t^\varepsilon) dt + \sqrt{2\varepsilon} g(x_t^\varepsilon) dW_t, \quad x_0 \in \mathbb{R}^d$$

- ▷ b, g Lipschitz continuous, bounded-growth condition
- ▷ $a(x) = g(x)g(x)^T \geq \frac{1}{M} \text{Id}$ (uniform ellipticity)

Infinitesimal generator \mathcal{A}^ε of diffusion x_t^ε

$$\mathcal{A}^\varepsilon v(t, x) = \varepsilon \sum_{i,j=1}^d a_{ij}(x) \frac{\partial^2}{\partial x_i \partial x_j} v(t, x) + \langle b(x), \nabla v(t, x) \rangle$$

Compare to Fokker–Planck operator: \mathcal{L}^ε is the adjoint operator of \mathcal{A}^ε

Approaches to the exit problem

- ▷ Mean first-exit times and locations via PDEs
- ▷ Exponential asymptotics via Wentzell–Freidlin theory

Diffusion exit from a domain: Relation to PDEs

Theorem

- ▷ Poisson problem:

$\mathbb{E}_x\{\tau_{\mathcal{D}}^\varepsilon\}$ is the unique solution of

$$\begin{cases} \mathcal{A}^\varepsilon u = -1 & \text{in } \mathcal{D} \\ u = 0 & \text{on } \partial\mathcal{D} \end{cases}$$

- ▷ Dirichlet problem:

$\mathbb{E}_x\{f(x_{\tau_{\mathcal{D}}^\varepsilon}^\varepsilon)\}$ is the unique solution of

(for $f : \partial\mathcal{D} \rightarrow \mathbb{R}$ continuous)

$$\begin{cases} \mathcal{A}^\varepsilon w = 0 & \text{in } \mathcal{D} \\ w = f & \text{on } \partial\mathcal{D} \end{cases}$$

Remarks

- ▷ Expected first-exit times and distribution of first-exit locations obtained **exactly** from PDEs

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- ▷ In principle . . .

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Remarks

- ▷ Expected first-exit times and distribution of first-exit locations obtained **exactly** from PDEs
- ▷ In principle . . .
- ▷ Smoothness assumption for $\partial\mathcal{D}$ can be relaxed to “exterior-ball condition”

An example in $d = 1$

Motion of a Brownian particle in a quadratic single-well potential

$$dx_t^\varepsilon = b(x_t^\varepsilon) dt + \sqrt{2\varepsilon} dW_t$$

where $b(x) = -\nabla V(x)$, $V(x) = ax^2/2$ with $a > 0$

- ▶ Drift pushes particle towards bottom
- ▶ Probability of x_t^ε leaving $\mathcal{D} = (\alpha_1, \alpha_2) \ni 0$ through α_1 ?

Solve the (one-dimensional) Dirichlet problem

$$\begin{cases} \mathcal{A}^\varepsilon w = 0 & \text{in } \mathcal{D} \\ w = f & \text{on } \partial\mathcal{D} \end{cases} \quad \text{with} \quad f(x) = \begin{cases} 1 & \text{for } x = \alpha_1 \\ 0 & \text{for } x = \alpha_2 \end{cases}$$

$$\mathbb{P}_x \{x_{\tau_D^\varepsilon}^\varepsilon = \alpha_1\} = \mathbb{E}_x f(x_{\tau_D^\varepsilon}^\varepsilon) = w(x) = \int_x^{\alpha_2} e^{V(y)/\varepsilon} dy \Big/ \int_{\alpha_1}^{\alpha_2} e^{V(y)/\varepsilon} dy$$

An example in $d = 1$: Small noise limit?

$$\mathbb{P}_x \{x_{T_D^\varepsilon} = \alpha_1\} = \int_x^{\alpha_2} e^{V(y)/\varepsilon} dy \Big/ \int_{\alpha_1}^{\alpha_2} e^{V(y)/\varepsilon} dy$$

What happens in the small-noise limit?

$$\lim_{\varepsilon \rightarrow 0} \mathbb{P}_x \{x_{T_D^\varepsilon} = \alpha_1\} = 1 \quad \text{if } V(\alpha_1) < V(\alpha_2)$$

$$\lim_{\varepsilon \rightarrow 0} \mathbb{P}_x \{x_{T_D^\varepsilon} = \alpha_1\} = 0 \quad \text{if } V(\alpha_2) < V(\alpha_1)$$

$$\lim_{\varepsilon \rightarrow 0} \mathbb{P}_x \{x_{T_D^\varepsilon} = \alpha_1\} = \frac{1}{|V'(\alpha_1)|} \Big/ \left(\frac{1}{|V'(\alpha_1)|} + \frac{1}{|V'(\alpha_2)|} \right) \quad \text{if } V(\alpha_1) = V(\alpha_2)$$

Large deviations: Wentzell–Freidlin theory

Exponential asymptotics via large deviations

- ▶ Probability of observing sample paths being close to a given function $\varphi : [0, T] \rightarrow \mathbb{R}^d$ behaves like $\sim \exp\{-2I(\varphi)/\varepsilon\}$
- ▶ Large-deviation rate function

$$I(\varphi) = I_{[0, T]}(\varphi) = \begin{cases} \frac{1}{2} \int_0^T \|\dot{\varphi}_s - b(\varphi_s)\|^2 ds & \text{for } \varphi \in \mathcal{H}_1 \\ +\infty & \text{otherwise} \end{cases}$$

- ▶ Large deviation principle reduces est. of probabilities to variational principle: For any set Γ of paths on $[0, T]$

$$-\inf_{\Gamma^o} I \leq \liminf_{\varepsilon \rightarrow 0} 2\varepsilon \log \mathbb{P}\{(x_t^\varepsilon)_t \in \Gamma\} \leq \limsup_{\varepsilon \rightarrow 0} 2\varepsilon \log \mathbb{P}\{(x_t^\varepsilon)_t \in \Gamma\} \leq -\inf_{\Gamma} I$$

- ▶ Assume domain \mathcal{D} has unique asymptotically stable equilibrium point x_-^*
- ▶ **Quasipotential** with respect to x_-^* = cost to reach z against the flow

$$V(x_-^*, z) := \inf_{t > 0} \inf \{I_{[0, t]}(\varphi) : \varphi \in \mathcal{C}([0, t], \mathcal{D}), \varphi_0 = x_-^*, \varphi_t = z\}$$

Wentzell–Freidlin theory

Theorem [Wentzell & Freidlin, 1969–72, 1984] For arbitrary initial condition in \mathcal{D}

- ▶ Mean first-exit time: $\mathbb{E}\tau_{\mathcal{D}}^{\varepsilon} \sim e^{\bar{V}/2\varepsilon}$ as $\varepsilon \rightarrow 0$
- ▶ Concentration of first-exit times

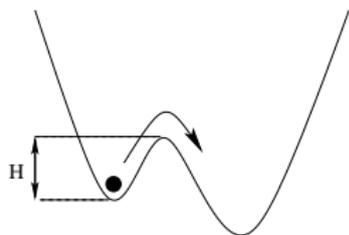
$$\mathbb{P}\left\{e^{(\bar{V}-\delta)/2\varepsilon} \leq \tau_{\mathcal{D}}^{\varepsilon} \leq e^{(\bar{V}+\delta)/2\varepsilon}\right\} \rightarrow 1 \text{ as } \varepsilon \rightarrow 0 \quad (\text{for arbitrary } \delta > 0)$$
- ▶ Concentration of exit locations near minima of quasipotential

Gradient case (reversible diffusion)

- ▶ $b = -\nabla V$, $g = \text{Id}$
- ▶ Quasipotential $V(x_{-}^{*}, z) = 2[V(z) - V(x_{-}^{*})]$
- ▶ Cost for leaving potential well is

$$\bar{V} = \inf_{z \in \partial \mathcal{D}} V(x_{-}^{*}, z) = 2[V(z^{*}) - V(x_{-}^{*})] = 2H$$
- ▶ Attained for paths going **against** the flow:

$$\dot{\varphi}_t = +\nabla V(\varphi_t)$$



Remarks

- ▶ **Arrhenius Law** [van't Hoff 1885, Arrhenius 1889] follows as a corollary

$$\mathbb{E}_{x_-^*} \tau_+ \simeq \text{const } e^{[V(z^*) - V(x_-^*)]/\varepsilon}$$

where $\tau_+ =$ **first-hitting time** of small ball $B_\delta(x_+^*)$ around other minimum x_+^*

$$\tau_+ = \tau_{x_+^*}^\varepsilon(\omega) = \inf\{t \geq 0: x_t^\varepsilon(\omega) \in B_\delta(x_+^*)\}$$

- ▶ Exponential asymptotics depends **only on barrier height**
- ▶ LDP also leads information on optimal transition paths
- ▶ **Only 1-saddles** are relevant for transitions between wells
- ▶ Multiwell case described by hierarchy of “cycles”
- ▶ Nongradient case: Work with variational problem
- ▶ Prefactor cannot be obtained by this approach

Subexponential asymptotics

Refined results in the gradient case: Kramers' law

First-hitting time of a small ball $B_\delta(x_+^*)$ around minimum x_+^*

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Arrhenius Law [van't Hoff 1885, Arrhenius 1889] – see previous slide

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$$\mathbb{E}_{x_-^*} \tau_+ \simeq \text{const} e^{[V(z^*) - V(x_-^*)]/\varepsilon}$$

Eyring–Kramers Law [Eyring 35, Kramers 40]

$$\triangleright d = 1: \quad \mathbb{E}_{x_-^*} \tau_+ \simeq \frac{2\pi}{\sqrt{|V'''(x_-^*)| |V''(z^*)|}} e^{[V(z^*) - V(x_-^*)]/\varepsilon}$$

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$$\triangleright d \geq 2: \quad \mathbb{E}_{x_-^*} \tau_+ \simeq \frac{2\pi}{|\lambda_1(z^*)|} \sqrt{\frac{|\det \nabla^2 V(z^*)|}{\det \nabla^2 V(x_-^*)}} e^{[V(z^*) - V(x_-^*)]/\varepsilon}$$

where $\lambda_1(z^*)$ is the unique negative eigenvalue of $\nabla^2 V$ at saddle z^*

Proving Kramers' law (multiwell potentials)

- ▶ Low-lying spectrum of generator of the diffusion (analytic approach) [Helffer & Sjöstrand 85, Miclo 95, Mathieu 95, Kolokoltsov 96, ...]
- ▶ Potential theoretic approach [Bovier, Eckhoff, Gaynard & Klein 04]

$$\mathbb{E}_{x_-^*} \tau_+ = \frac{2\pi}{|\lambda_1(z^*)|} \sqrt{\frac{|\det \nabla^2 V(z^*)|}{\det \nabla^2 V(x_-^*)}} e^{[V(z^*) - V(x_-^*)]/\varepsilon} [1 + \mathcal{O}((\varepsilon |\log \varepsilon|)^{1/2})]$$

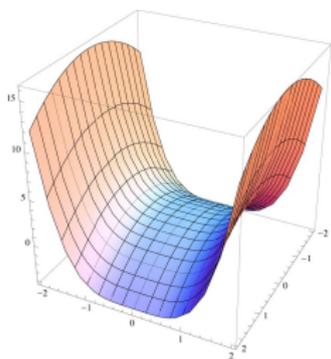
- ▶ Full asymptotic expansion of prefactor [Helffer, Klein & Nier 04]
- ▶ Asymptotic distribution of τ_+ [Day 83, Bovier, Gaynard & Klein 05]

$$\lim_{\varepsilon \rightarrow 0} \mathbb{P}_{x_-^*} \{ \tau_+ > t \cdot \mathbb{E}_{x_-^*} \tau_+ \} = e^{-t}$$

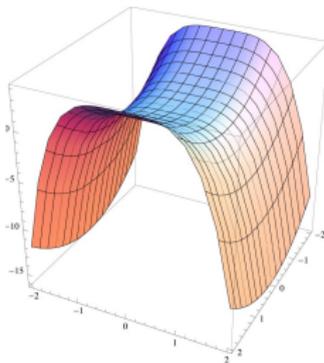
Generalizations: Non-quadratic saddles

What happens if $\det \nabla^2 V(z^*) = 0$?

- $\det \nabla^2 V(z^*) = 0 \Rightarrow$ At least one vanishing eigenvalue at saddle z^*
 \Rightarrow Saddle has at least one **non-quadratic** direction
 \Rightarrow Kramers Law not applicable



Quartic unstable direction



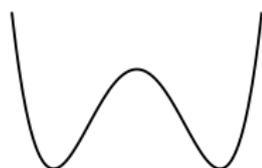
Quartic stable direction

Why do we care about this non-generic situation?

Parameter-dependent systems may undergo **bifurcations**

Example: Two harmonically coupled particles

$$V_\gamma(x_1, x_2) = U(x_1) + U(x_2) + \frac{\gamma}{2}(x_1 - x_2)^2$$

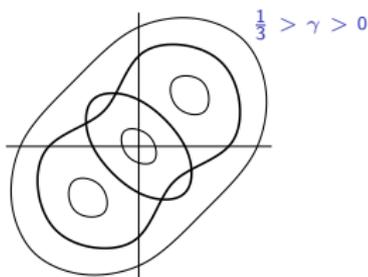
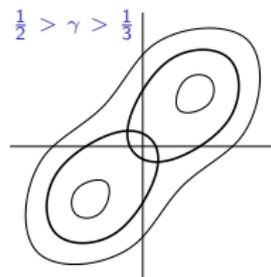
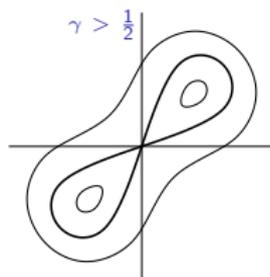


$$U(x) = \frac{x^4}{4} - \frac{x^2}{2}$$

Change of variable: Rotation by $\pi/4$ yields

$$\widehat{V}_\gamma(y_1, y_2) = -\frac{1}{2}y_1^2 - \frac{1-2\gamma}{2}y_2^2 + \frac{1}{8}(y_1^4 + 6y_1^2y_2^2 + y_2^4)$$

Note: $\det \nabla^2 \widehat{V}_\gamma(0,0) = 1 - 2\gamma \Rightarrow$ Pitchfork bifurcation at $\gamma = 1/2$



Transition times for non-quadratic saddles

- ▶ Assume x_-^* is a quadratic local minimum of V (non-quadratic minima can be dealt with)
- ▶ Assume x_+^* is another local minimum of V
- ▶ Assume $z^* = 0$ is the **relevant** saddle for passage from x_-^* to x_+^*
- ▶ Normal form near saddle

$$V(y) = -u_1(y_1) + u_2(y_2) + \frac{1}{2} \sum_{j=3}^d \lambda_j y_j^2 + \dots$$

- ▶ Assume growth conditions on u_1, u_2

Theorem [Berglund & G, 2010])

$$\mathbb{E}_{x_-^*} \tau_+ = \frac{(2\pi\varepsilon)^{d/2} e^{-V(x_-^*)/\varepsilon}}{\sqrt{\det \nabla^2 V(x_-^*)}} \bigg/ \varepsilon \frac{\int_{-\infty}^{\infty} e^{-u_2(y_2)/\varepsilon} dy_2}{\int_{-\infty}^{\infty} e^{-u_1(y_1)/\varepsilon} dy_1} \prod_{j=3}^d \sqrt{\frac{2\pi\varepsilon}{\lambda_j}}$$

$$\times [1 + \mathcal{O}((\varepsilon|\log \varepsilon|)^\alpha)]$$

where $\alpha > 0$ depends on the growth conditions and is explicitly known

Corollary: Pitchfork bifurcation

Pitchfork bifurcation:
$$V(y) = -\frac{1}{2}|\lambda_1|y_1^2 + \frac{1}{2}\lambda_2 y_2^2 + C_4 y_2^4 + \frac{1}{2} \sum_{j=3}^d \lambda_j y_j^2 + \dots$$

- ▷ For $\lambda_2 > 0$ (possibly small wrt. ε):

$$\mathbb{E}_{x_-^*} \tau_+ = 2\pi \sqrt{\frac{(\lambda_2 + \sqrt{2\varepsilon C_4}) \lambda_3 \dots \lambda_d}{|\lambda_1| \det \nabla^2 V(x_-^*)}} \frac{e^{[V(z^*) - V(x_-^*)]/\varepsilon}}{\Psi_+(\lambda_2/\sqrt{2\varepsilon C_4})} [1 + R(\varepsilon)]$$

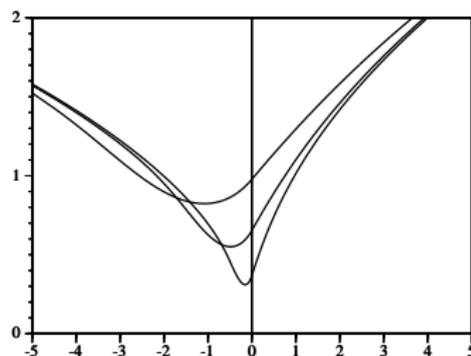
where

$$\Psi_+(\alpha) = \sqrt{\frac{\alpha(1+\alpha)}{8\pi}} e^{\alpha^2/16} K_{1/4}\left(\frac{\alpha^2}{16}\right)$$

$$\lim_{\alpha \rightarrow \infty} \Psi_+(\alpha) = 1$$

$K_{1/4}$ = modified Bessel fct. of 2nd kind

- ▷ For $\lambda_2 < 0$: Similar, involving $I_{\pm 1/4}$



$\lambda_2 \mapsto$ prefactor

$\varepsilon = 0.5, \varepsilon = 0.1, \varepsilon = 0.01$

Cycling

New phenomena in non-gradient case: Cycling

Simplest situation of interest:

Nontrivial invariant set which is a single periodic orbit

Assume from now on:

$d = 2$, $\partial\mathcal{D} = \text{unstable}$ periodic orbit

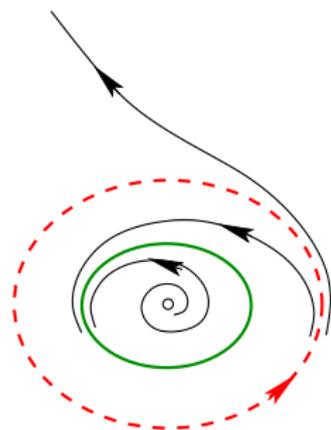
- ▷ $\mathbb{E}\tau_{\mathcal{D}} \sim e^{\bar{V}/2\epsilon}$ still holds
- ▷ Quasipotential $V(\Pi, z) \equiv \bar{V}$ is constant on $\partial\mathcal{D}$:
Exit equally likely anywhere on $\partial\mathcal{D}$ (on exp. scale)
- ▷ Phenomenon of **cycling** [Day '92]:

Distribution of $x_{\tau_{\mathcal{D}}}$ on $\partial\mathcal{D}$ does not converge as $\epsilon \rightarrow 0$

Density is *translated* along $\partial\mathcal{D}$ proportionally to $|\log \epsilon|$.

- ▷ In *stationary regime*: (obtained by reinjecting particle)

Rate of escape $\frac{d}{dt} \mathbb{P}\{x_t \notin \mathcal{D}\}$ has $|\log \epsilon|$ -periodic prefactor [Maier & Stein '96]



Universality in cycling

Theorem ([Berglund & G '04, '05, work in progress])

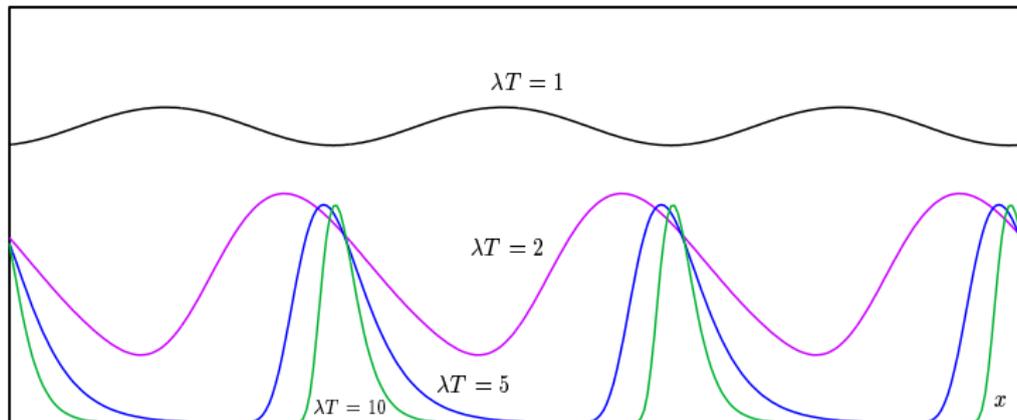
There exists an explicit parametrization of $\partial\mathcal{D}$ s.t. the exit time density is given by

$$p(t, t_0) = \frac{f_{\text{trans}}(t, t_0)}{\mathcal{N}} Q_{\lambda T}(\theta(t) - \frac{1}{2}|\log \varepsilon|) \frac{\theta'(t)}{\lambda T_{\text{K}}(\varepsilon)} e^{-(\theta(t) - \theta(t_0)) / \lambda T_{\text{K}}(\varepsilon)}$$

- ▷ $Q_{\lambda T}(y)$ is a *universal* λT -periodic function
- ▷ $\theta(t)$ is a “natural” parametrisation of the boundary:
 - $\theta'(t) > 0$ is explicitly known *model-dependent*, T -periodic fct.;
 - $\theta(t + T) = \theta(t) + \lambda T$
- ▷ $T_{\text{K}}(\varepsilon)$ is the analogue of Kramers' time: $T_{\text{K}}(\varepsilon) = \frac{C}{\sqrt{\varepsilon}} e^{\bar{V}/2\varepsilon}$
- ▷ f_{trans} grows from 0 to 1 in time $t - t_0$ of order $|\log \varepsilon|$

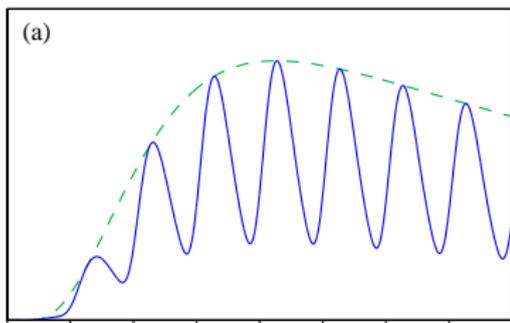
The universal profile

$$y \mapsto Q_{\lambda T}(\lambda T y) / 2\lambda T$$

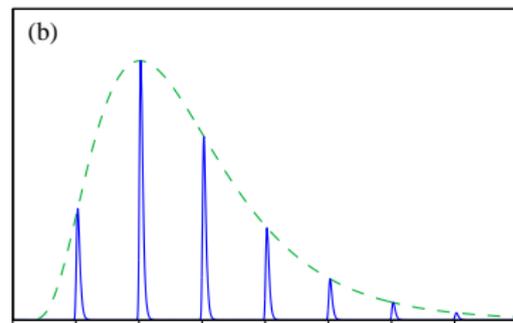


- ▶ Profile determines **concentration of first-passage times** within a period
- ▶ Shape of peaks: Gumbel distribution $P(z) = \frac{1}{2} e^{-2z} \exp\left\{-\frac{1}{2} e^{-2z}\right\}$
- ▶ The larger λT , the more pronounced the peaks s
- ▶ For smaller values of λT , the peaks overlap more

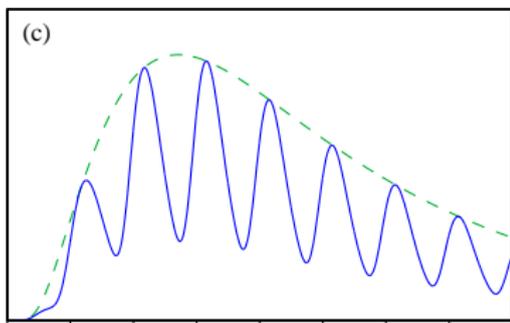
Density of the first-passage time for $\bar{V} = 0.5$, $\lambda = 1$



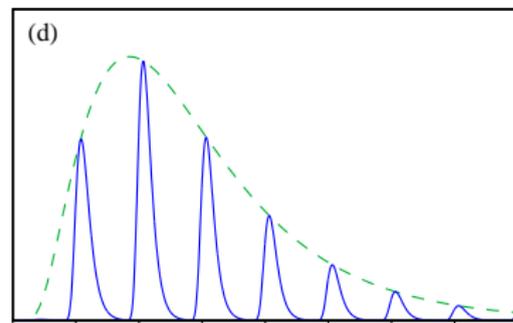
$\varepsilon = 0.4$, $T = 2$



$\varepsilon = 0.4$, $T = 20$



$\varepsilon = 0.5$, $T = 2$



$\varepsilon = 0.5$, $T = 5$

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