“Lévy flights in steep potential wells: Langevin modeling versus direct response to energy landscapes”

(Piotr Garbaczewski, Opole, Poland)

Somewhat puzzling topic: Reflecting boundary data for Lévy – stable processes

Fractional Laplacians in bounded domains: Killed, reflected, censored, and taboo Lévy flights PRE 99, 04126, (2019)

Qery: Is there a problem ?

Lévy flights versus Lévy walks in bounded domains [Dybiec, Gudowska-Nowak, Barkai, Dubkov; Phys. Rev. E 95, 052102, (2017)]

Lévy flights in extremally steep potential wells and in an infinitely deep rectangular well (regarded as a limit case), whose impenetrable boundaries are interpreted as reflecting.

The pertinent boundary conditions are visualised on the path-wise level, in terms of the Langevin equation for large (even) *n* and compared with the results of the simulated free random motion with ***stopping*** or ***wrapping*** conditions at the boundaries at $x = \pm L$.

$$\frac{dx}{dt} = -V_n'(x) + \zeta_\alpha(t).$$

n even and large, eventually

$$\lim_{n\to\infty} V_n(x) = \lim_{n\to\infty} \frac{1}{n}\frac{|x|^n}{L^n}$$

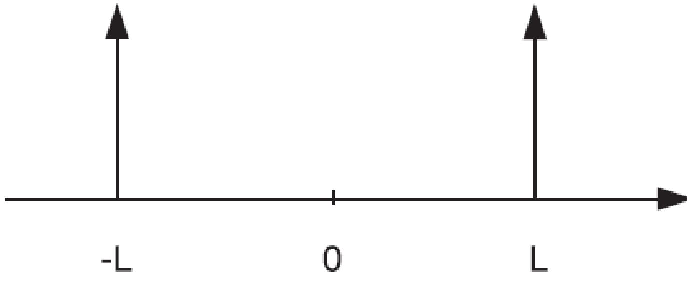
$$\dot{x} = b(x) + A^\mu(t) \Rightarrow \partial_t\rho = -\nabla(b\rho) - \lambda|\Delta|^{\mu/2}\rho$$

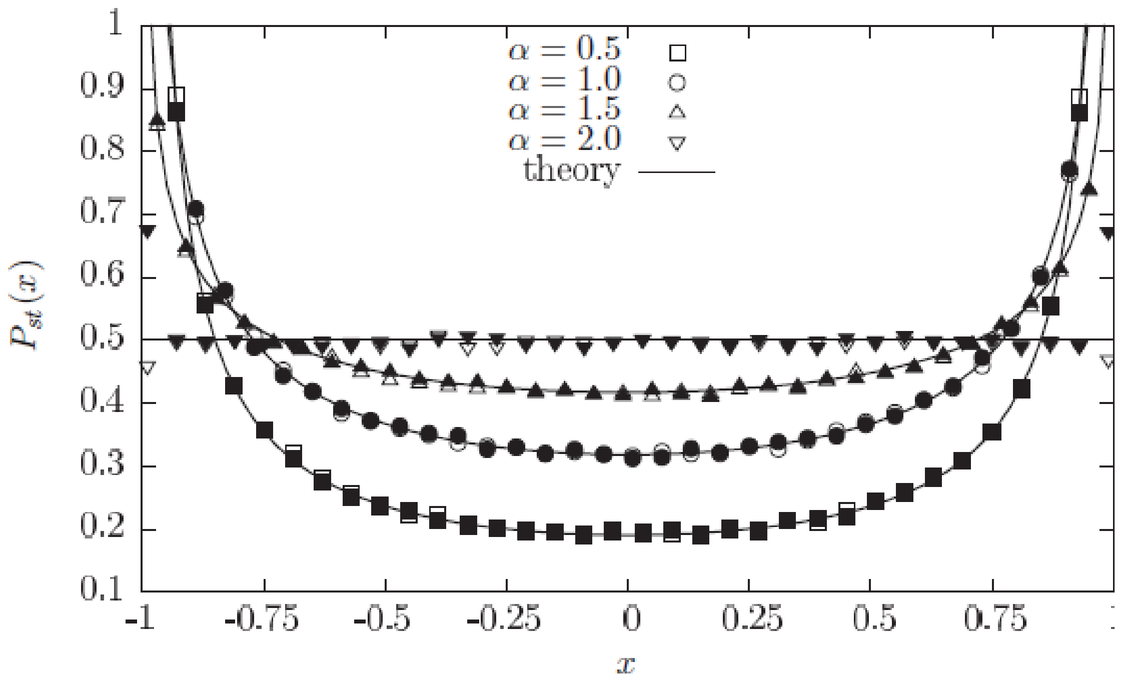
μ and α in use interchangeably

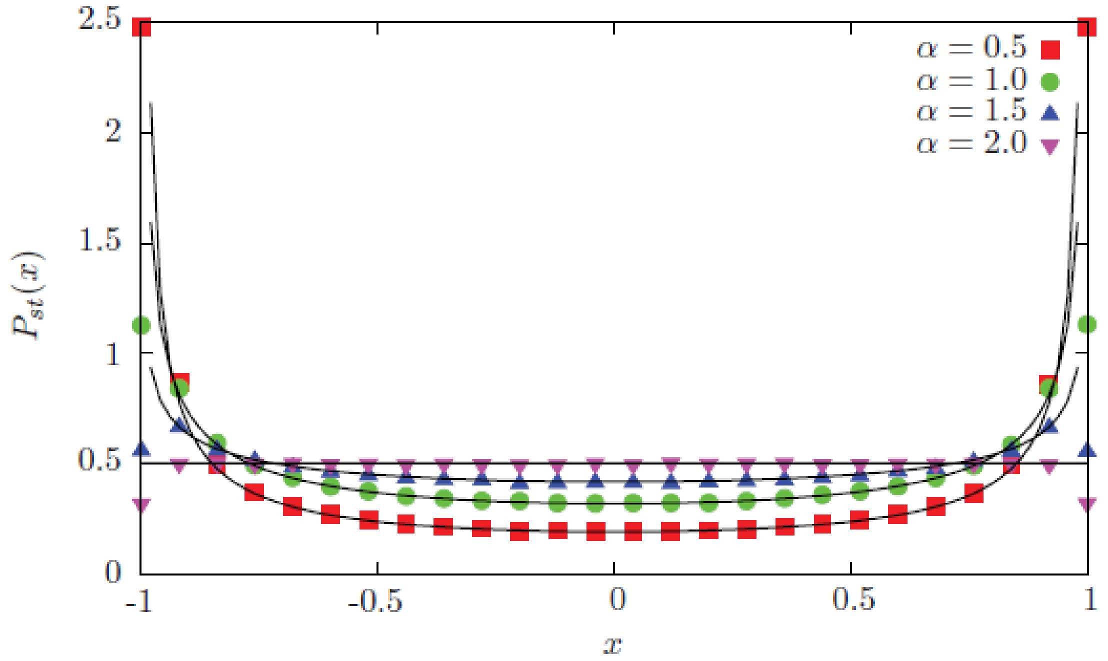
Limiting (?) steady state pdf is expected to conform with the formula due to Denisov, Horsthemke, Hänggi, PRE 77, 061112,(2008)

Warning: the convergence is not uniform

$$P_{\mathrm{st}}(x) = \frac{\Gamma(\alpha)(2L)^{1-\alpha}(L^2 - x^2)^{\alpha/2-1}}{\Gamma^2(\alpha/2)}.$$







Left panel: Filled points correspond to the **confining** potential $V_{800}(x)$, empty points refer to the **stopping** scenario. (L=1).

What about the wrapping scenario ?

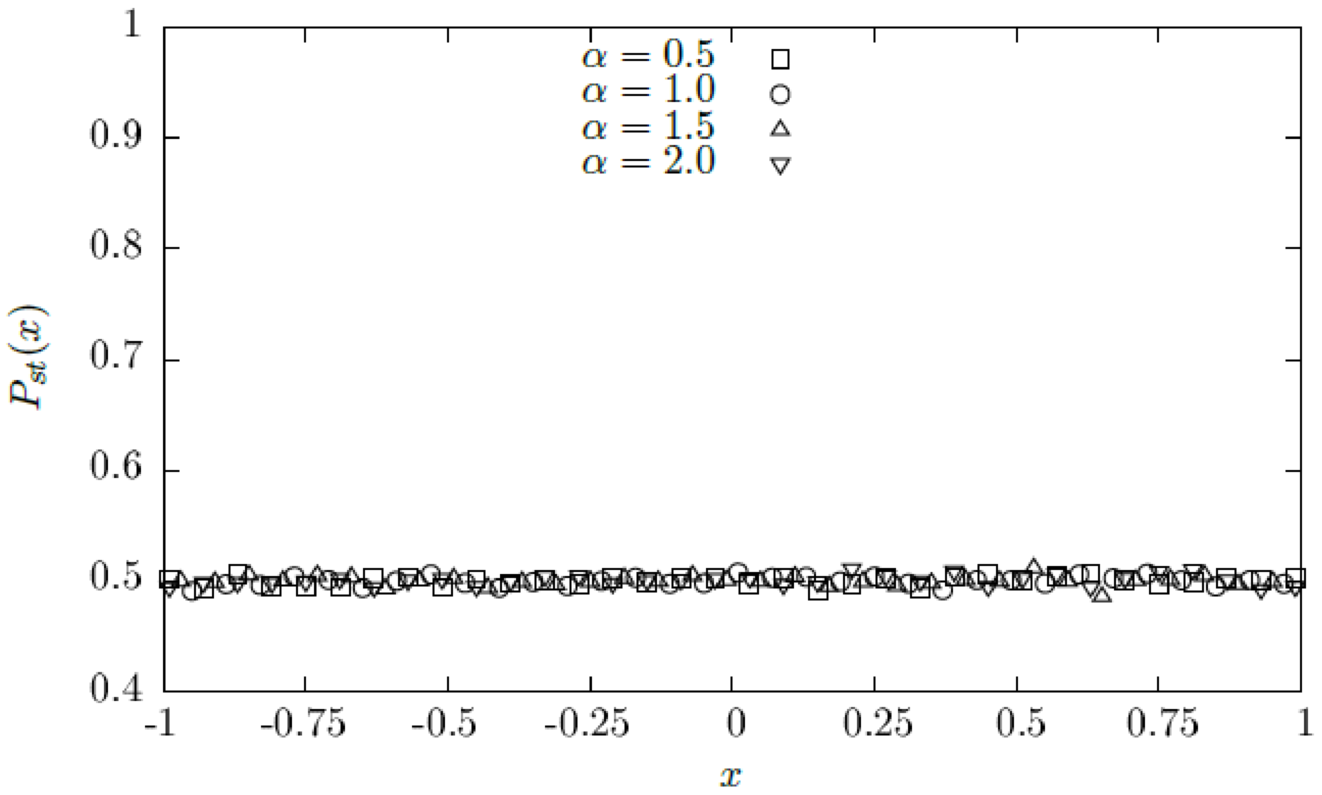
three different realizations of the reflecting condition:

(i) Motion reversal: A trajectory that ends at $x < -L$ is wrapped around the left boundary, i.e., $x \to -L + |x + L|$.

(ii) Motion stopping: A trajectory that crosses $-L$ is paused at $-L + \varepsilon$, where ε is a small and positive parameter. The point $-L + \varepsilon$ is used as a starting point for a next jump.

(iii) Motion confined within a potential: The reflecting boundary can be implemented by considering the motion in a bounding potential,

The **wrapping (motion reversal)** scenario, irrespective of the stability index value $0 < \alpha \leq 2$, **results in uniform** stationary states for the (otherwise free) Lévy motion, while restricted by impenetrable boundaries. !



(B. Dybiec, private communication)

Nonlocal operator, generator of the Lévy-stable proces, 0<α<2

$$(-\Delta)^{\alpha/2} f(x) = \mathcal{A}_{\alpha,n} \lim_{\varepsilon \to 0^+} \int_{R^n \supset \{|y-x|>\varepsilon\}} \frac{f(x)-f(y)}{|x-y|^{\alpha+n}} dy,$$

$$-|\Delta|^{\mu/2} \equiv \frac{\partial^\mu}{\partial |x|^\mu}$$

$$\mathcal{A}_{\alpha,n} = \frac{2^\alpha \Gamma\left(\frac{\alpha+n}{2}\right)}{\pi^{n/2} |\Gamma\left(-\frac{\alpha}{2}\right)|} = \frac{2^\alpha \alpha \Gamma\left(\frac{\alpha+n}{2}\right)}{\pi^{n/2} \Gamma\left(1-\frac{\alpha}{2}\right)}$$

$$n \geqslant 1$$

We shall mostly refer to the 1D (i.e. n=1) case

$$\partial_t \rho = -\nabla\left(-\frac{\nabla V}{m\beta}\rho\right) - \lambda |\Delta|^{\mu/2} \rho$$

Reference form of the fractional F-P equation

We consider the F-P eq. with the identically vanishing drift term, while restricted to the open interval, e. g. to x in (-1,1)

$$\partial_t f(x,t) = -(-\Delta)^{\alpha/2} f(x,t)$$

We admit functions f(x,t) with the property **f(x,t)=0 for all** $|x| \geq 1$ (for convenience we set L=1) and address the existence issue of a time-independent solution (with the L(R) normalization being implicit) of the equation

Not only a pseudo-differential equation, refers to **the spectral problem on the interval !**

$$(-\Delta)^{\alpha/2} f(x,t) = 0$$

for x in (-1,1)

The solution has been known to mathematicians, quite independently of the original Denisov, Horsthemke, Hänggi argument (2008) and involves the concept of **a singular α - harmonic function.**

Example 3.3. *Let $\alpha < 2$. Suppose that D is the open unit ball in $\mathbb{R}^d$. Then the function*

$$f(x) = (1 - |x|^2)^{\alpha/2-1}, \quad |x| < 1$$

$$f(x) = 0, \quad |x| \geq 1$$

is α-harmonic in D and

$$\lim_{x \to Q \in \partial D} f(x) = \infty.$$

Note: A function f(x) is α– harmonic on an open set D, if and only if f is C^2 on D and $\boxed{(-\Delta)^{\alpha/2} f(x,t) = 0}$

Denisov at al.: probability density on D

$$\boxed{\rho_\alpha(x) = (2)^{1-\alpha} \frac{\Gamma(\alpha)}{\Gamma^2(\alpha/2)} (1 - x^2)^{\alpha/2-1}}$$

for the Cauchy case i.e. α =1, we have in (-1,1)

$$\rho_1(x) = \frac{1}{\pi} \frac{1}{\sqrt{1 - x^2}}$$

Important ! These densities need to be considered on the whole of R, and required to vanish beyond D = (-1,1)

Remark (minor detour): Lévy processes with **killing/absorption** at the boundaries of the open set D involve a **spectral solution and a related spectral definition of the transition density**:

$$\begin{cases} -(-\Delta)^{\alpha/2}\varphi_n(x) = -\lambda_n \varphi_n(x) & x \in D \\ \varphi_n(x) = 0, & x \in D^c \end{cases}$$

$$0 < \lambda_1 < \lambda_2 \leqslant \lambda_3 \leqslant \dots$$

$$\lambda_n = \left[\frac{n\pi}{2} - \frac{(2-\alpha)\pi}{8}\right]^\alpha - O\left(\frac{2-\alpha}{n\sqrt{\alpha}}\right)$$

Kwaśnicki, (2012))

$$\boxed{k_D(t,x,y) = \sum_{n=1}^{\infty} e^{-\lambda_n t}\, \phi_n(x)\, \phi_n(y)}$$

$$T_t^D f(x) = E^x[f(X_t); t < \tau_D] = \int_D k_D(t,x,y) f(y) \mathrm{d}y$$

The major technical difference, if compared with the previous **zero-eigenvalue problem**, is quite subtle and reduces to the demand that for a function f(x, t), the boundary (**Dirichlet**) value 0 must be reached continuously from the interior D of the closed set, and this property must be shared by $(-\Delta)^{\alpha/2} f(x,t)$ as well.

The above spectral problem on the interval [-1,1] is equivalent to that of **the infinitely deep rectangular well with** the **exterior Dirichet** boundary data i. e. for all x in R\(-1,1)

Problem: no analogous (explicit) **spectral solution** is known for the **reflecting case** (with zero as the bottom eigenvalue) for Lévy flights

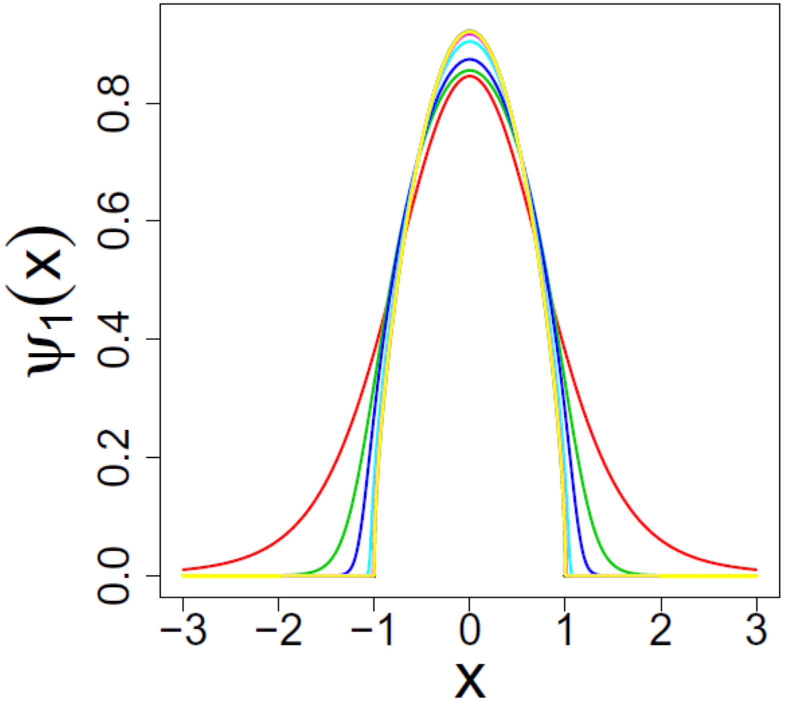
Motivations for further discussion

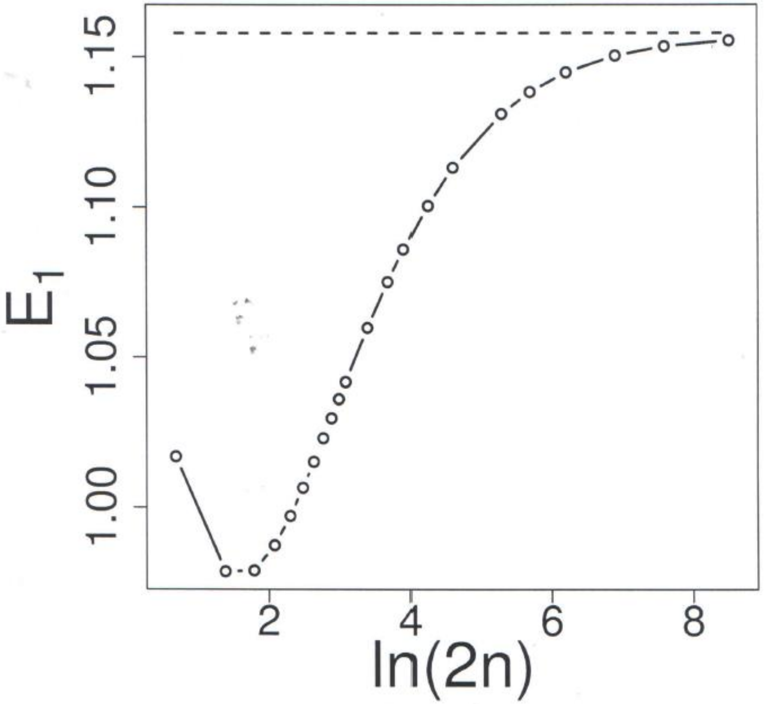
(i) In the **Cauchy case**, we have worked out an approximation procedure of the **Dirichlet infinite well** spectral problem **by a sequence of Hamiltonian problems with the Cauchy operator plus a steep anharmonic potential**, whose even exponent m=2n is allowed to approach infinity (the higher the maximum in the figure below, the better an approximation of the true ground-state function is)

$$\boxed{H\psi_1 = \lambda_1 \psi_1}$$

$$\boxed{H = |\Delta| + x^{2n}}$$

n=1, 4, 10, 50, 250, up to 2500





Reliable for not too small n

Problem: No analogous spectral result is in existence for the reflecting infnite well; the latter can be sequentially approximated by following the direct **Langevin route** (c.f. Dubkov et al.)

(ii) Targeted stochasticity and reverse egineering problem:

The Eliazar-Klafter targeted stochasticity concept , together with that of the reverse engineering (reconstruction of the stochastic process once a **target pdf is a priori given**), has been originally devised for **Lévy-driven Langevin systems**

Eliazar and Klafter, (2003): „how to design a **Langevin** system, subject to a given Lévy noise, that would yield a pre-specified ‘‘target’’ steady state behavior”

Our **reverse engineering proposal** [Pre84, 011142, (2011)], with roots in papers by Brockmann and Sokolov (2002-2003), refers to the **non-Langevin alternative**, e.g. the „potential landscape idea**”: given a probability density function and the (Lévy) driver, specify the semigroup potential, and the jump-type dynamics for which this pdf is actually a long-time asymptotic (target) solution of the master equation.**

(iii) Related issue of detailed balance:

Lévy targeting and the principle of detailed balance PHYSICAL REVIEW E **84**, 011142 (2011)

The detailed balace has been found not to hold true in case of **Langevin driven Levy flights** (Kuśmierz, Dybiec, Gudowska-Nowak, (2018)). However, it does hold true in the **non-Langevin** alternative !

Detailed balance - preserving Lévy processes and related Lévy semigroups

$$\partial_t \rho = -\lambda |\Delta|^{\mu/2} \rho$$

$$(|\Delta|^{\mu/2} f)(x) = -\frac{\Gamma(\mu+1)\sin(\pi\mu/2)}{\pi} \int \frac{f(z)-f(x)}{|z-x|^{1+\mu}}\, dz$$

$$\partial_t \rho(x) = \int [w(x|z)\rho(z) - w(z|x)\rho(x)]\nu_\mu(dz)$$

we replace the jump rate $w(x|y) \sim 1/|x-y|^{1+\mu}$ by the expression $w_\phi(x|y) \sim \frac{\exp[\Phi(x)-\Phi(y)]}{|x-y|^{1+\mu}}$

$$\rho_* = \exp(2\Phi)$$

$$\rho(x,t) \to \rho_*(x)$$

$$(1/\lambda)\partial_t \rho = |\Delta|_\Phi^{\mu/2} f = -\exp(\Phi)\, |\Delta|^{\mu/2} [\exp(-\Phi)\rho] + \rho \exp(-\Phi)|\Delta|^{\mu/2} \exp(\Phi)$$

$$\rho_*(x) = (1/Z)\exp(-V_*(x)/k_B T)$$

Gibbs-Boltzmann form

$$\partial_t \rho = -\exp(-\kappa V_*/2)\, |\Delta|^{\mu/2} \exp(\kappa V_*/2)\rho + \rho \exp(\kappa V_*/2)|\Delta|^{\mu/2} \exp(-\kappa V_*/2), \;\; \kappa = 1/k_B T.$$

This dynamics is manifestly non-Langevin by construction, and **is Lévy semigroup – driven.** Namely, define

$$\boxed{\hat{H}_\mu \equiv \lambda|\Delta|^{\mu/2} + \mathcal{V}(x)}$$

with the ground state condition

$$\boxed{\hat{H}_\mu \rho_*^{1/2} = 0}$$

The semigroup dynamics is ruled by the equation

$$\boxed{\partial_t \Psi = -\hat{H}_\mu \Psi = -\lambda|\Delta|^{\mu/2}\Psi - \mathcal{V}(x)\Psi\,,}$$

$$\boxed{\mathcal{V} = -\lambda\, \frac{|\Delta|^{\mu/2}\rho_*^{1/2}}{\rho_*^{1/2}}}$$

This potential actually sets an „energy landscape" (Feynman-Kac formula related concept)

$$k(y,s,x,t) = \int \exp\left[-\int_s^t \mathcal{V}(X(u),u)\,du\right] d\mu[s,y\mid t,x]$$

Clearly, given a predefined square root of the stationary pdf, while setting $\Psi(x,t) = \rho(x,t)\,\rho_*^{-1/2}(x)$

we arrive at the equation which controls a relaxation of the time- dependent pdf towards a stationary one

$$\boxed{\rho(x,t) \to \rho_*(x)}$$

$$\boxed{\partial_t \rho = \lambda[-\rho_*^{1/2}|\Delta|^{\mu/2}(\rho_*^{-1/2}\,\cdot\,) + \rho_*^{-1/2}(|\Delta|^{\mu/2}\rho_*^{1/2})]\,\rho}$$

This relaxation proces is paralleled by $\boxed{\psi(x,t) \to \rho_*^{1/2}}$

Response to external forces in the Langevin scenario

$$\dot{x} = b(x) + A^{\mu}(t) \Longrightarrow \partial_t \rho = -\nabla(b \cdot \rho) - \lambda|\Delta|^{\mu/2}\rho$$

Assume per force that $\rho_*(x) = (1/Z)\exp(-V_*(x)/k_B T)$ might arise as a stationary solution of the fractional Fokker-Planck equation, hence in the large time asymptotic of the Langevin-induced dynamics.

$$b(x) = -\lambda \frac{\int |\Delta|^{\mu/2} \rho_*(x)\, dx}{\rho_*(x)}$$

Eliazar-Klafter version employs Fourier transforms

Targeted stochasticity

The drift b(x) **cannot** be represented in the form $-\nabla V_*(x)$ (up to a multiplicative constant); Eliazar-Klafter no-go statement (2003)

Targeted stochasticity for the Cauchy driver (potential landscape issue made explicit)

$$(|\nabla|f)(x) = -\frac{1}{\pi}\int \frac{f(z)-f(x)}{|z-x|^2}\,dz$$

Link with logarithmic potentials

ln ($\sigma^2 + x^2$)

Ornstein-Uhlenbeck-Cauchy process

Langvin route, F-P Eq.

$$\boxed{\partial_t \rho = -\lambda|\nabla|\rho + \nabla[(\gamma x)\rho]}$$

$$\boxed{\rho_*(x) = \frac{\sigma}{\pi(\sigma^2 + x^2)}}$$

$\sigma = \frac{\lambda}{\gamma}$,

In below set μ=1

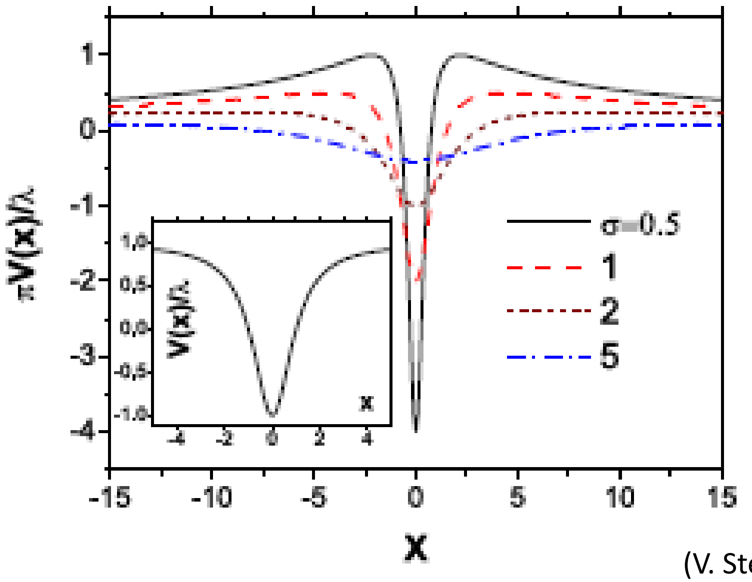
Invariant density vs semigroup potential

„energy landscape”

$$\boxed{\mathcal{V} = -\lambda \frac{|\Delta|^{\mu/2}\,\rho_*^{1/2}}{\rho_*^{1/2}}}$$

$$\mathcal{V}(x) = \frac{\lambda}{\pi}\left[-\frac{2}{\sqrt{a}} + \frac{x}{a}\ln\frac{\sqrt{a}+x}{\sqrt{a}-x}\right]$$

$\boxed{a = \sigma^2 + x^2}$



$$\boxed{\hat{H}_\mu \equiv \lambda|\Delta|^{\mu/2} + \mathcal{V}(x).}$$

(V. Stephanovich –coll.)

We recall the title of the talk: **“Lévy flights in steep potential wells: Langevin modeling versus direct response to energy landscapes”.**

We revisit the problem of Lévy motion in steep potential wells, addressed in [A.A. Kharcheva et al., J. Stat Mech., (2016), 054029] and [B. Dybiec et al. , PRE 95, 05201, (2017)] and **discuss the alternative semigroup (Feynman-Kac) motion scenario.**

Langevin route: sequential approximation (n goes to infinity) of an infinite well with **reflecting walls**

The infinite rectangular potential well with impenetrable boundaries located at $x = \pm L$ can be obtained as $n \to \infty$ limit of the symmetric single-well potential

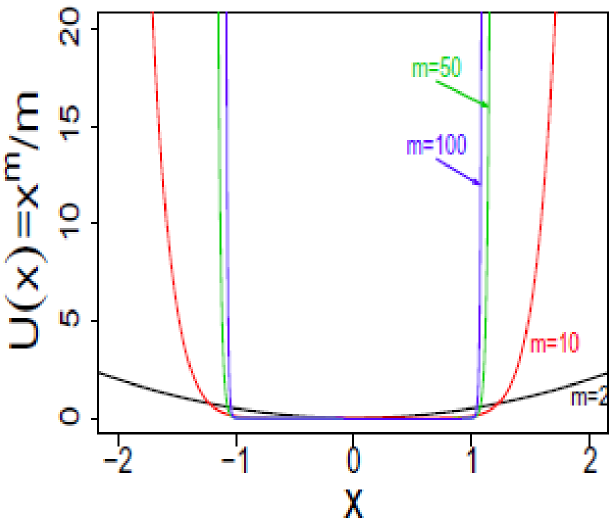
$$V_n(x) = \frac{(x/L)^{2n}}{2n}$$

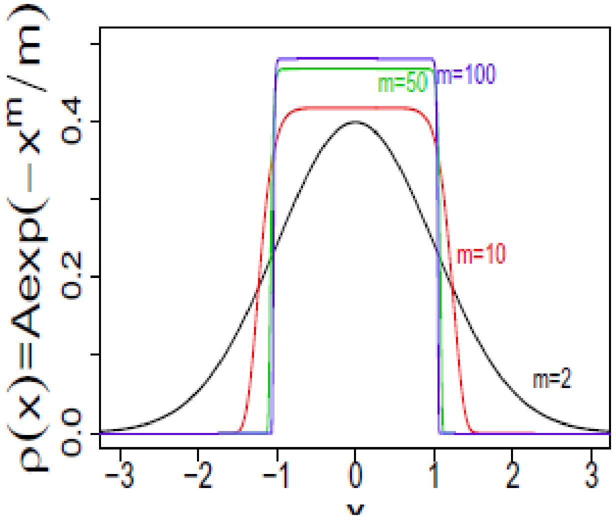
The very same folk phrase refers to the reflecting and Dirichlet infinite well

for which stationary states for $\alpha = 1$ are also known

(Dubkov, Spagnolo et al. - somewhat involved but explicit analytic formula)

Sequential approximation, with m=2n growing





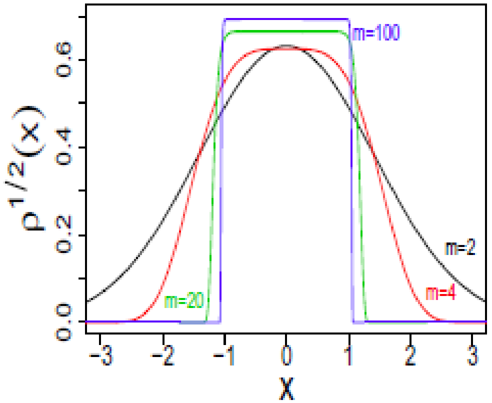
Langevin-Wiener scenario (Brownian motion)

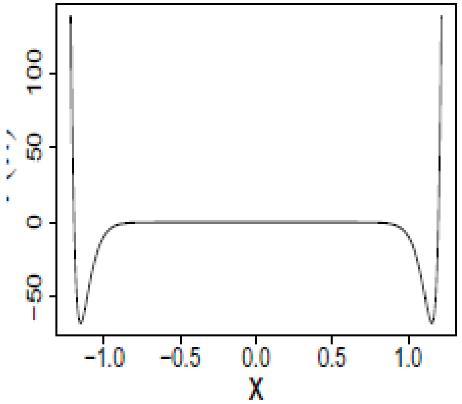
$$\partial_t \rho = D\Delta\rho - \nabla\,(b\cdot\rho)\,.$$

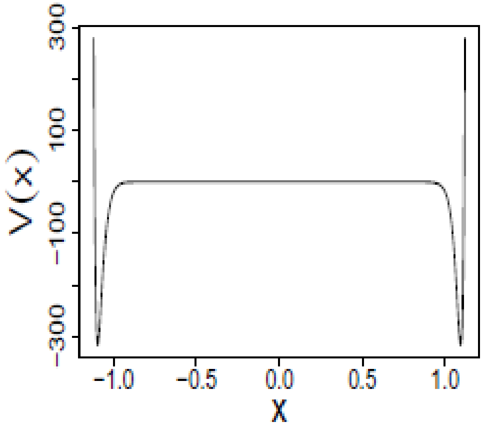
$$\rho(x) = A\,\exp[-U(x)],\ \text{with}\ 1/A = \int_{-\infty}^{+\infty} \exp[-U(x)]\,dx$$

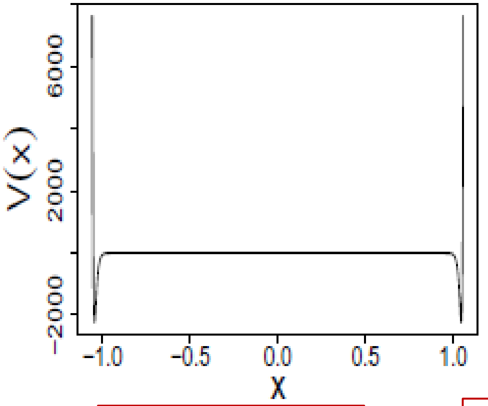
This Boltzmann-Gibbs pdf is our $\rho_*(x)$

Feynman-Kac semigroup potential landscape









$\mathcal{V}$

$\rho_*^{1/2}(x)$ is an eigenfunction of $-\Delta + \mathcal{V}(x)$ corresponding to the eigenvalue zero,

$\hat{H}_\mu \rho_*^{1/2} = 0$

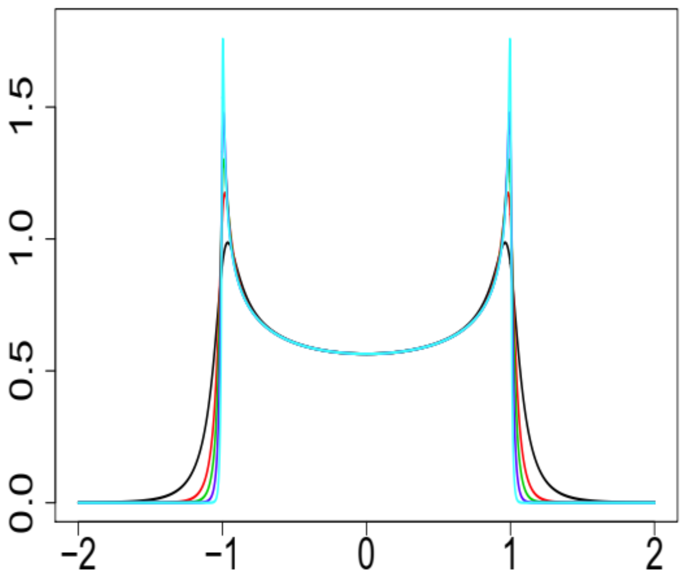
μ= 2

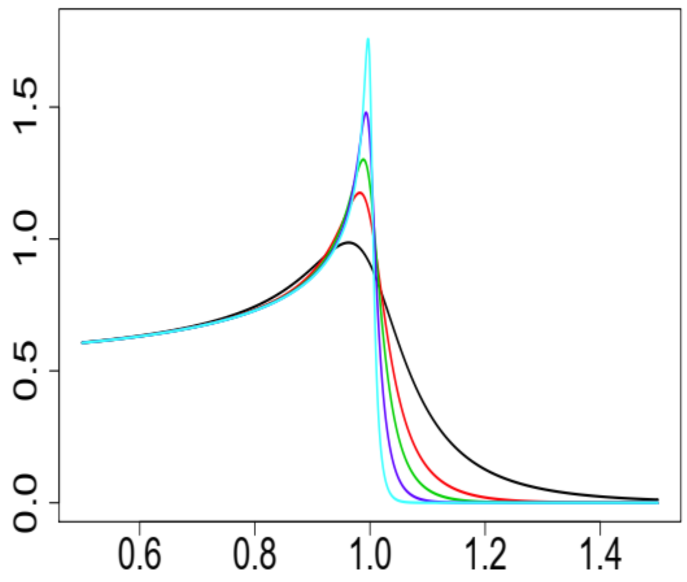
$$\mathcal{V}(x) = \mathcal{V}_m(x) = \frac{x^{m-2}}{2}\left[\frac{x^m}{2} + (1-m)\right]\ \text{for}\ m = 20, 40, 100.$$

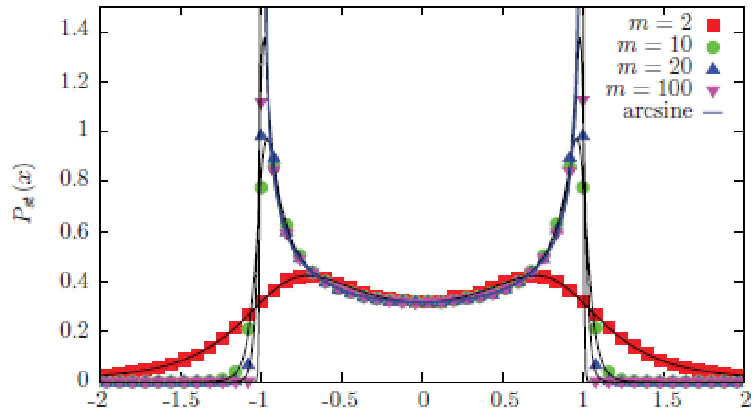
$\partial_t\Psi = \Delta\Psi - \mathcal{V}\Psi = -\hat{H}\Psi$

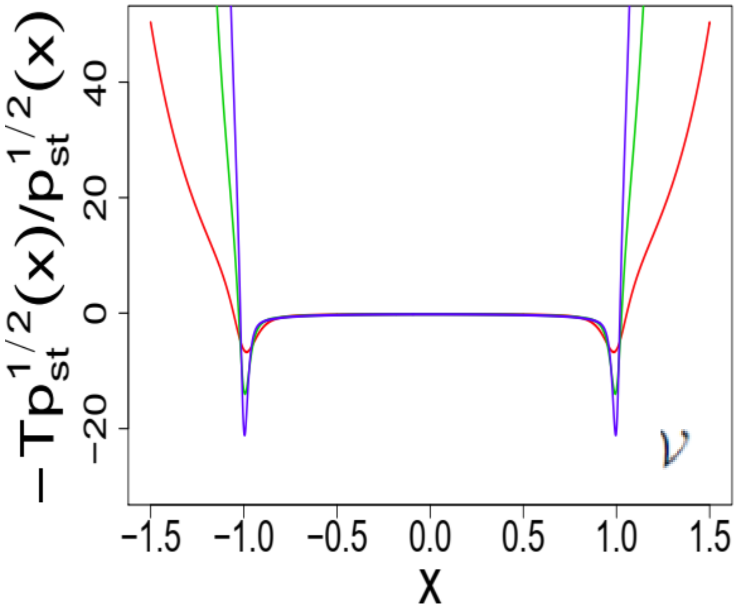
Minima of the semigroup potential are located at points $x = \pm[(m-2)/2]^{1/m}$ i.e. $|x| \sim m^{1/m} > 1$.

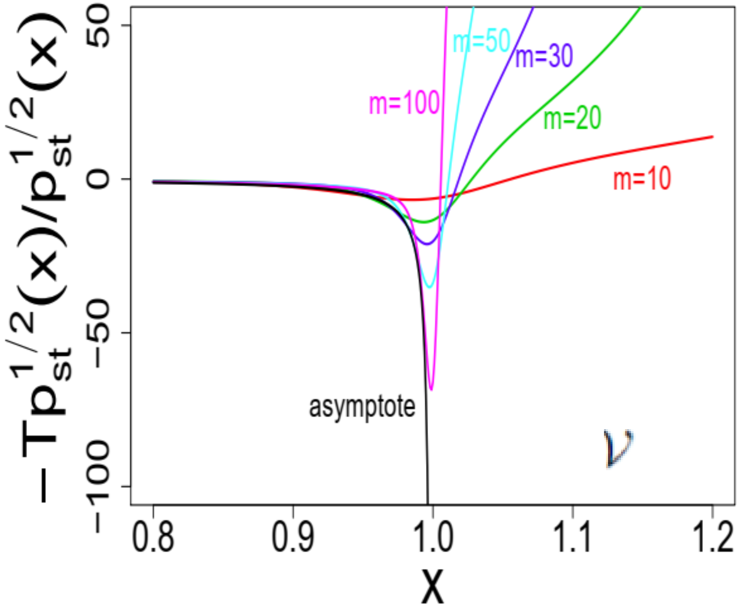
Langevin-Cauchy scenario – target pdfs from which $\rho_*^{1/2}$ and $\mathcal{V}$ are inferred to set the „potential landscape", Cauchy semigroup view. m= 10, 20, 30, 50, 100











Cauchy semigroup potential

$$\mathcal{V} = -\lambda \frac{|\Delta|^{\mu/2} \rho_*^{1/2}}{\rho_*^{1/2}}$$

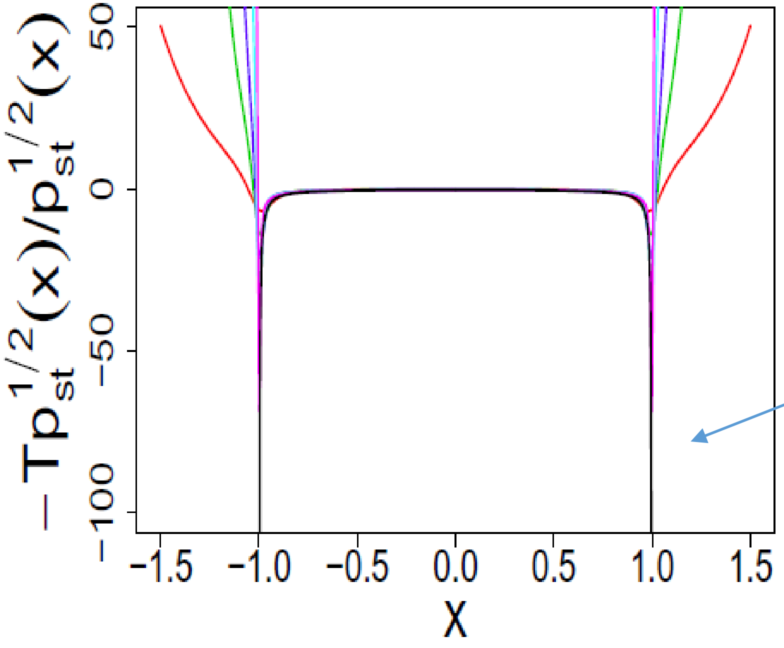
μ=1
λ= 1

Black curve refers to the **square root** of the limiting pdf $\rho_1(x) = \frac{1}{\pi} \frac{1}{\sqrt{1-x^2}}$ i.e.:

$\rho_*^{1/2}$(x) = $p_{st}^{1/2}(x) = \frac{1}{\sqrt{\pi \sqrt{1-x^2}}}$

m=10, 20, 30

$\boxed{\hat{H}_\mu \equiv \lambda |\Delta|^{\mu/2} + \mathcal{V}(x).}$ $\boxed{\hat{H}_\mu \rho_*^{1/2} = 0}$ $\boxed{\mu = 1}$



The asymptotic potential is non-positive (turned upside down).
Is that strange ?

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$$(-\Delta)^{\alpha/2} f(x) = \left[(-\Delta)^{\alpha/2}_{D,\mathrm{reg}} + \kappa_D(x)\right] f(x)$$

vhere $\kappa_D(x) = \mathcal{A}_{\alpha,n} \int_{R^n \setminus D} |x-y|^{-(n+\alpha)} dy$ is non-negative

spectral problem for the regional fractional Laplacian in $D = [-1, 1]$

$$(-\Delta)^{\alpha/2}_{D,\mathrm{reg}} \psi(x) = (-\Delta)^{\alpha/2} \psi(x) - \kappa^{\alpha}_{D}(x) \psi(x) = E\psi(x)$$

$$-A_\alpha \int_{-1}^{1} \frac{\psi(u)du}{|u-x|^{1+\alpha}} - \frac{A_\alpha \psi(x)}{\alpha} \frac{(1-x)^\alpha + (1+x)^\alpha}{(1-x^2)^\alpha} = E\psi(x)$$

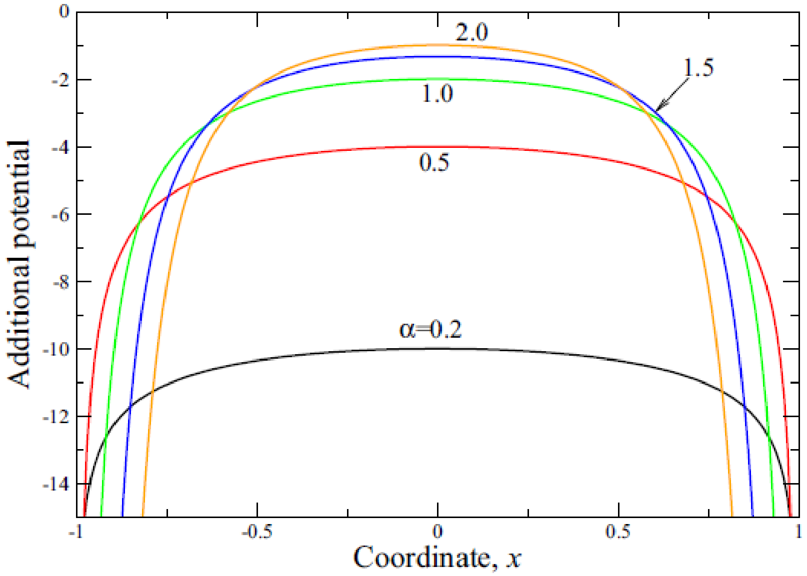

FIG. 1. Negative-definite singular potential (32) in the spectral problem for the regional fractional Laplacian for various values of α (figures near curves).

Last sentence of the Abstract: Our focus is on a link with the problem of boundary data (Dirichlet versus Neumann, or absorbing versus reflecting) for the Lévy motion and its generator on the interval (or bounded domain, in general*).*

At the moment we have no definite and unambiguos answer concerning the **detailed spectral relationship** of the motion generator on the interval with reflecting boundary data, with that of the affiliated semigroup, neither in the Brownian nor in the Lévy context. **This work is in progress.**

Brownian reference to the term „spectral"

$$\partial_t f(x) = \Delta_{\mathcal{N}} f(x)$$

Laplacian on a closed interval [a,b], with Neumann boundary data

$$(\partial_x f)(a) = 0 = (\partial_x f)(b)$$

Eigenfunction expansion of the transition probability density (**meaning of the term „spectral"**)

$$\boxed{k_{\mathcal{N}}(t,x,y) = \frac{1}{\mathrm{vol}(D)} + \sum_{n=1}^{\infty} e^{-\kappa_n t}\, \psi_n(x)\, \psi_n(y)}$$

$$\boxed{\psi_0(x) = 1/\sqrt{\mathrm{vol}(D)}}$$

Phys. Rev. E **99**, 042126 (2019) **Fractional Laplacians in bounded domains: Killed, reflected, censored, and taboo Lévy flights** Piotr Garbaczewski and Vladimir Stephanovich

arXiv:1906.06694 **Brownian motion in trapping enclosures: Steep potential wells and false bistability of affiliated Schrödinger type systems** Piotr Garbaczewski and Mariusz Żaba