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Hypocoercive relaxation to equilibrium for some kinetic models *via* a third order differential inequality

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Abstract

This paper deals with the study of some particular kinetic models, where the randomness acts only on the velocity variable level. Usually, the Markovian generator cannot satisfy any Poincaré's inequality. Hence, no Gronwall's lemma can easily lead to the exponential decay of F_t (the L^2 norm of a test function along the semi-group). Nevertheless for the kinetic Fokker-Planck dynamics and for a piecewise deterministic evolution we show that F_t satisfies a third order differential inequality which gives an explicit rate of convergence to equilibrium.

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1 Introduction

In order to improve MCMC algorithms one can try to resort to higher order dynamics which, for instance kinetic ones. Indeed, non-reversible dynamics possess naturally more inertia than reversible ones and have less tendency to turn back and hesitate than the simple reversible process. This is an important issue for the escape of local minima and such non-reversible processes may then converge faster to equilibrium (cf. [12], [11], [36], [37]).

For instance, [37] compare numerically the following sampling procedures of the Gibbs measure $e^{-U(x)} dx$ associated to a potential U . First, thanks to the Fokker-Planck dynamics

$$dX_t = -U'(X_t) + \sigma dB_t$$

and secondly with the kinetic Fokker-Planck one (shorten from now on to kFP ; it is called Langevin dynamics in [37], but we stick here to [8] for the denomination)

$$\begin{cases} dX_t = Y_t dt \\ dY_t = -U'(X_t)dt - Y_t dt + \sqrt{2}dB_t \end{cases} \quad (1)$$

where B_t stands for a standard brownian motion. It turns out, numerically, that the second one is generally more efficient, in the sense that it converges faster toward the steady regime.

About a decade ago, there were no method to obtain explicit rates of convergence for non-reversible Markov process, as usually the classical functional inequality theory (cf. [1], [33]), powerfull in reversible settings, does not apply. But since then, as the topic is of interest in many fields, many different approaches have emerged. Here is a far from exhaustive list of references roughly sorted in three group : first the analytical method based on the spectral study of hypoelliptical operators, initiated by Hérau and Nier (in [29], followed by [28], [18], [27], [31]), where the decay is obtained in some Sobolev norm. Secondly the probabilistic method of coupling *à la* Meyn and Tweedie, in Wasserstein distances (see [23],[16],[26], [5], and [2] for a link with functional inequalities), recently succesfully applied in particular in the field of PDMPs (piecewise deterministic Markovian processes ; see [3], [21], [7], [4]). Finally the method of the modified Lyapunov function initiated by Desvillettes and Villani ([9], [8], [10], [40],[39], [35], [19], [6]), and then refined by Dolbeault, Mouhot and Schmeiser ([14], [15], [25], [24]) who work for the latter with a norm equivalent to the L^2 one, without any addition of supplementary derivatives. The present work is rather close to this last approach.

Despite (or thanks to) all this work, some phenomena arising from the interplay between the deterministic transport and the stochastic part of the generator still deserve to be better understood. In particular the convergence to equilibrium appears to be inhomogeneous in time: in [22], where the L^2 distance $d(t)$ between the distribution at time t and the equilibrium is explicitly computed for the kFP process with a quadratic potential, the decay is flat for small times, *i.e.* $d(t) \simeq 1 - ct^3$. Indeed, if $d'(0)$ were non zero, it would imply a Poincaré inequality (see [1]) but none is satisfied there. Furthermore in some cases we have $d(t) = g_t e^{-\lambda t}$ for some $\lambda > 0$ but with a periodic prefactor g_t . Such oscillations, linked to the competition for the convergence to equilibrium between the position and the velocity (see the discussion p.66 of [9]), have also been numerically observed for the Boltzmann equation in [20]. This behaviour is reminiscent of functions of the form $\phi(t) = e^{-\lambda t} (a + b \cos(\nu t + \theta))$, which are solutions of

$$((\partial_t + \lambda)^3 + \nu^2(\partial_t + \lambda)) \phi = 0.$$

The third order may also be linked to the number of Lie Brackets one has to take in Hörmander's hypoellipticity theory to obtain a full rank (cf. [30]), and is expected to get bigger for higher order models (for instance oscillator chains [17]). Yet most of the current results rely on the existence of some quantity that somehow decreases *at all time*, in other words in a first order differential equation (with the notable exception of [38] where the usual dissipation of entropy is checked in mean in time). We can expect, in fact, a third order differential inequality to be satisfied, which can account for these inhomogeneities. This is the scope of the present article. This is not a new idea (cf. [8], [32]) but up to our knowledge it had never been succesfully completed. In fact for the kFP model it has been noted in [22] that no linear combination of the L^2 norm and its three first derivatives can be non-positive for all test functions, so we will clarify in the sequel the meaning of third order differential inequality.

The models

More precisely, this work will be devoted to study the relaxation to equilibrium for two kinetic models. The dynamics of the first one, the kFP process, is given by equation (1).

$(X_t, Y_t) \in \mathbb{R}^2$ is then the position-speed process of a particle in a potential U with friction and noise. Results about its convergence to equilibrium can be found in [22] for a quadratic potential, and, according to one favorite method, [28], [16] or [8] (among others) for more general cases (the coupling method, in [16], only deals with convex potentials).

The second one is a generalised version of the telegraph process, for which $(X_t, Y_t) \in \mathbb{R} \times \{\pm 1\}$, where $dX_t = Y_t dt$ and Y_t jumps to its opposite following an inhomogeneous rate $a(X_t, Y_t)$. Here the particle go forward at constant speed and only does U-turn (cf. Figure 1 and 2 for an illustration). In the classical telegraph process the rate of jump a is constant over its definition space. If we take $X_t \in \mathbb{R}/2\pi\mathbb{Z}$ to ensure ergodicity, we obtain maybe one of the simplest toy models for kinetic processes, cited as a basic example in [19] or [15] and precisely studied in [34]. When the rate is no longer constant, the underlying algebra collapses. An ergodic version on the real line has recently been investigated in [21] but, again with coupling method, the invariant measure corresponds to a convex potential.

In our cases, (X_t, Y_t) has a unique invariant measure denoted μ . Recall that the semi-group $(P_t)_{t \geq 0}$ of operators on $L^2(\mu)$ is defined by

$$P_t f(x, y) := \mathbb{E}(f(X_t, Y_t) | X_0 = x, Y_0 = y).$$

Its infinitesimal generator L is

$$L f := \lim_{t \rightarrow 0} \frac{L^2(\mu) P_t f - f}{t}$$

for f such that the limit exists. To focus on other questions, from now on we assume the existence of a core \mathcal{D} dense in $L^2(\mu)$, stable by L , and we will always consider $f \in \mathcal{D}$. For a more analytical setting of the problem, denoting by \hat{L} the dual of L , which operates on measures, the law μ_t of (X_t, Y_t) is the (weak) solution of

$$\begin{cases} \partial_t \mu_t = \hat{L} \mu_t \\ \mu_0 = \text{law}(X_0, Y_0). \end{cases}$$

Then

$$P_t f(x, y) = \int f(u, v) \mu_t(du, dv)$$

when $\mu_0 = \delta_{(x, y)}$. We aim to quantify the convergence of μ_t to μ .

For the kFP model, $\mu = e^{-U(x)} dx \otimes e^{-\frac{y^2}{2}} dy$ is the Gibbs measure associated to the Hamiltonian $U(x) + \frac{y^2}{2}$, and

$$L f = y \partial_x f - U'(x) \partial_y f - y \partial_y f + \partial_y^2 f. \quad (2)$$

For the telegraph one, $\mu = e^{-U(x)} dx \otimes \frac{\delta_1 + \delta_{-1}}{2}(dy)$ where $U'(x) = a(x, 1) - a(x, -1)$ (see Lemma 6). Denoting $f_-(x, y) = f(x, -y)$,

$$L f = y \partial_x f + a(x, y)(f_- - f). \quad (3)$$

These two processes share some common features. One of them is that there is no coercivity from the deterministic part of the dynamics when the potential is not convex; in other words two particles coupled with the same random part don't have any trend to get closer. In the other hand the randomness only occurs in the velocity variable, and thus the processes are fully degenerate in the sense of [2] and their Bakry-Emery curvature (definition 5.3.4 in [1]) is equal to $-\infty$.

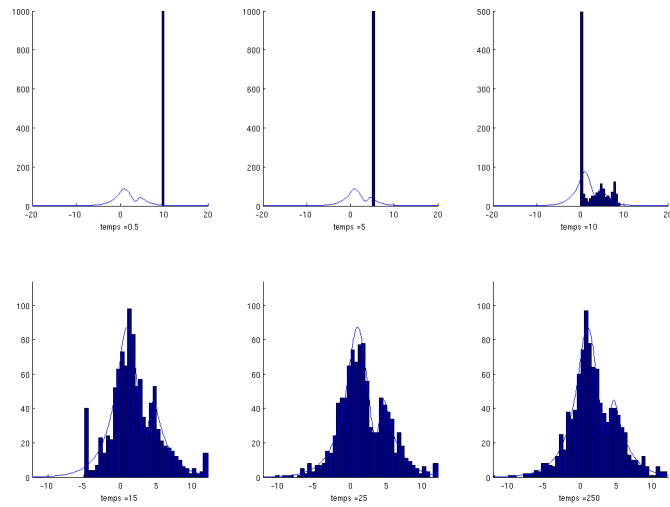


Figure 1: First marginal of the telegraph process at different time with a bi-modal invariant law $e^{-U(x)}dx$, $(X_0, Y_0) = (7, -1)$ and $a(x, y) = (yU'(x))_+$. While the potential decreases along the trajectory, the process is deterministic. It escapes easily from the local minimum.

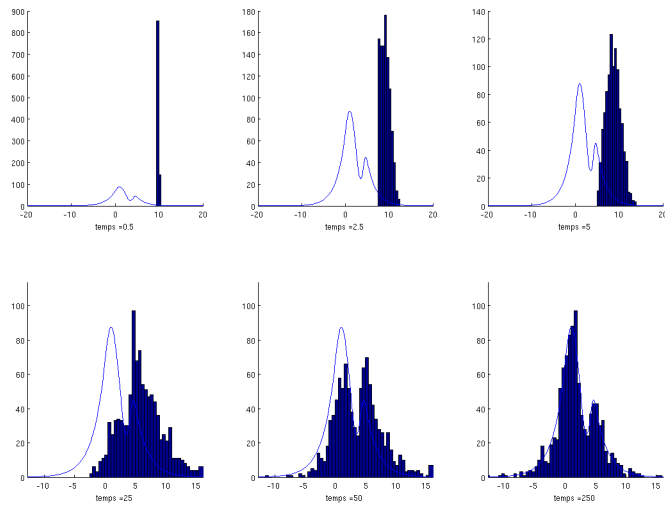


Figure 2: Here $a(x, y) = 1 + (yU'(x))_+$. In other words, contrary to Figure 1, there is always a minimal level of randomness : the behaviour is more diffusive and it takes longer to leave the local minimum.

Main result

Let $f_t = (P_t - \mu)f$, so that $\forall t \geq 0, \mu f_t = 0$; in other words $f_t \in 1^\perp$ the orthogonal space of the constants in $L^2(\mu)$. Let $F_t = \|f_t\|_{L^2(\mu)}^2$. In the following (cf. Section 2) we show that, under some assumptions on the potential U or on the rate a , there exist explicit $\lambda, \eta > 0$ and $\nu_* \in \mathbb{R}$ with $\mathcal{R}e(\eta - \sqrt{-\nu_*}) > 0$ and a function $t \mapsto \nu_t \geq \nu_*$ such that

$$(\partial_t + \lambda) \left[(\partial_t + \eta)^2 + \nu_t \right] F_t \leq 0. \quad (4)$$

Then exponential decay follows from the next result.

Theorem 1. *Assume (4) holds.*

- if $\nu_* \leq 0$ then $F_t \leq \phi_t$
- if $\nu_* > 0$ then $F_t \leq \phi_t + e^{-\eta t} \sup_{s \leq t} e^{\eta s} (\phi_s - F_s)$; furthermore the length of a time interval where $F > \phi$ is less than $\frac{\pi}{\nu_*}$

with in both cases ϕ solution of

$$(\partial_t + \lambda) \left[(\partial_t + \eta)^2 + \nu_* \right] \phi_t = 0,$$

$\phi_0 = F_0, \phi'_0 = F'_0$ and ϕ''_0 explicit. In particular,

$$\lim_{t \rightarrow \infty} \frac{1}{t} \ln F_t \leq -\min(\lambda, \mathcal{R}e(\eta - \sqrt{-\nu_*}))$$

Remark 1. • $\nu_* \leq 0$ can always be assumed.

- For $\nu_* > 0$, ϕ presents damped oscillations with a period $\frac{2\pi}{\nu_*}$ and a magnitude of order $e^{-\eta t}$. The theorem shows that F is interlaced with ϕ : F can be above ϕ but only if it's already been under, and not for too long.
- This does not give a bound for the operator norm of the semi-group in L^2 . As will be seen in the sequel, $\phi''(0)$ depends on $F''(0)$ and $\|\partial_x f_0\|^2$, which can be arbitrarily large with $F_0 = 1$ (we could obtain a bound by using estimates from the pseudodifferential calculus theory, but our aim was to avoid resorting to this powerful tool and to stay very elementary). The result in [14] does the job with no derivative - but not exactly with the L^2 norm; it could be possible to do the same in the present work.

Proof. The Gronwall lemma gives

$$\left[(\partial_t + \eta)^2 + \nu_* \right] F_t \leq \left[(\partial_t + \eta)^2 + \nu_t \right] F_t \leq \left(\left[(\partial_t + \eta)^2 + \nu_t \right] F_t \right)_{t=0} e^{-\lambda t} := C_0 e^{-\lambda t}.$$

Let ϕ be the solution of

$$\begin{cases} \left[(\partial_t + \eta)^2 + \nu_* \right] \phi = C_0 e^{-\lambda t} \\ \phi_0 = F_0, \phi'_0 = F'_0. \end{cases}$$

Thus

$$\left[(\partial_t + \eta)^2 + \nu_* \right] (F_t - \phi_t) \leq 0.$$

In the case where $\nu_* \leq 0$, using twice the Gronwall lemma gives

$$\begin{aligned} (\partial_t + \eta - \sqrt{-\nu_*})(\partial_t + \eta + \sqrt{-\nu_*})(F_t - \phi_t) &\leq 0 \\ \Rightarrow (\partial_t + \eta + \sqrt{-\nu_*})(F_t - \phi_t) &\leq 0 \\ \Rightarrow F_t - \phi_t &\leq 0. \end{aligned}$$

So now assume $\nu_* > 0$ and define $h_t = e^{\eta t} (F_t - \phi(t))$, so that $h'_t + \nu_* h_t \leq 0, h_0 = h'_0 = 0$. Define $M_t = \sup \{-h_s, 0 \leq s \leq t\}$ so that $h_t \geq -M_t$. M_t is always nondecreasing and it is

constant while h is increasing. Let us show that $h_t \leq M_t$ at every time. Assume it is false and consider $s = \inf\{t > 0, h_t > M_t\}$. M_t is constant for t in a neighborhood of s , $h_{s-\varepsilon} < M_s$ and $h_{s+\varepsilon} > M_s$ for $\varepsilon > 0$ small enough. So, as $h_s'' \leq -\nu_* h_s < 0$, necessarily $h_s' > 0$, which leads to $(h_s')^2 + \nu_* h_s^2 > \nu_* M_s^2$. Now consider $u = \sup\{0 \leq t \leq s, h_t' \leq 0\}$ (which exists if s exists, as $h_0'' \leq 0$) and note that $M_u = M_s$. We get $(h_u')^2 + \nu_* h_u^2 = \nu_* h_u^2 \leq \nu_* M_u^2$. Yet for $t \in (u, s]$, $h_t' > 0$ so

$$h_t' (h_t'' + \nu_* h_t) = \frac{1}{2} \frac{d}{dt} ((h_t')^2 + \nu_* h_t^2) \leq 0$$

and we've reached a contradiction.

Concerning the length of an interval where $F > \phi$, in other words where $h > 0$, define on this interval $\delta_t = -\frac{1}{h_t} (h_t'' + \nu_* h_t) \geq 0$. Thus h_t is solution of

$$\psi_t'' + (\nu_* + \delta_t)\psi_t = 0$$

and so vanish, according to the Sturm-Liouville comparison theorem (cf. [13] for instance), between two successive zeros of $\cos(\nu_* t + \theta)$ for any θ . \square

In Section 2, the kFP and telegraph models are proven to satisfy an inequality of the form (4). Section 3 is devoted to numerical studies, whose conclusion is that the method can give the good order of magnitude for the exponential rate of convergence, but shouldn't be trusted to compute parameters which accurately give the asymptotically fastest convergence. Finally an appendix gather the proof of the technical lemmas used throughout this work.

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2 Third order inequality

We start with considerations applying to both models. To compute the derivatives of F_t , we'll split L in its symmetric and anti-symmetric part. More precisely, if A and B are operators on $L^2(\mu)$, we denote by A^* the dual operator of A and by $[A, B]$ the Lie Brackets $AB - BA$. \langle, \rangle stands for the scalar product on $L^2(\mu)$.

Lemma 1. *Assume*

$$L = K + R - R^*$$

with $K^* = K$. Then

$$\begin{aligned} F_t' &= \langle (2K)f_t, f_t \rangle \\ F_t'' &= \langle (2K)^2 f_t, f_t \rangle + 4 \langle [K, R]f_t, f_t \rangle \\ F_t''' &= \langle (2K)^3 f_t, f_t \rangle + 12 \langle [K^2, R]f_t, f_t \rangle + 4 \langle [[K, R], R - R^*]f_t, f_t \rangle. \end{aligned}$$

The proof is given in the appendix.

As in kinetic models the coercive part K of L only acts on the velocity variable, one cannot find any $\lambda > 0$ such that, for all f_t , $F_t' \leq -\lambda F_t$. We call μ_1 (resp. μ_2) the first (resp. second) marginal of μ , namely the position (resp. velocity) distribution at equilibrium. In our specific models we'll have $\mu = \mu_1 \otimes \mu_2$. We call $V = Ker(\mu_2 - 1)$ the set of functions which does not depend on y . The orthogonal projection to V and V^\perp will be respectively denoted by π_V and π_\perp :

$$\pi_V f(x, y) = \mathbb{E}(f(x, Z) | Z \sim \mu_2) = \int f(x, z) \mu_2(dz), \quad \pi_\perp = 1 - \pi_V.$$

We will note $f_V = \pi_V f_t$ and $f_\perp = \pi_\perp f_t$; as f_V only depends on x we will sometimes consider f_V as a one-parameter function in $L^2(\mu_1)$. Finally let $G_t = \|\partial_x f_t\|^2$, and recall that a measure ν is said to satisfy a Poincaré (or spectral gap) inequality with constant c if

$$\int |\partial_z g(z)|^2 d\nu(z) \geq c \int |g(z)|^2 d\nu(z) \quad (5)$$

whenever $\nu g = 0$.

Lemma 2. *We have $\mu_1 f_V = 0$. In particular, if μ_1 satisfies a Poincaré inequality with constant c , we have*

$$G_t \geq \|\partial_x f_V\|^2 \geq c \|f_V\|^2$$

If furthermore $F'_t \leq -d \|f_\perp\|^2$ then

$$\frac{1}{F'_t} \left(G_t - \frac{c}{d} F'_t \right) \geq c$$

Proof. For the first assertion,

$$\begin{aligned} \int f_V(x) d\mu_1(x) &= \int \left(\int f_t(x, y) d\mu_2(y) \right) d\mu_1(x) \\ &= \mu f_t \\ &= 0. \end{aligned}$$

Furthermore $\partial_x^* \partial_x$ is self-adjoint and stabilizes V , so it stabilizes V^\perp and

$$G_t = \|\partial_x(f_V + f_\perp)\|^2 = \|\partial_x f_V\|^2 + \|\partial_x f_\perp\|^2 \geq \|\partial_x f_V\|^2.$$

Then $G_t - \frac{c}{d} F'_t \geq c F_t$ is clear. \square

Now we will show that in both models, the inequality (4) holds for some parameters.

2.1 The kinetic Fokker-Planck process

In this section (from Lemma 3 to Theorem 2) the generator is

$$L = y \partial_x - U'(x) \partial_y - y \partial_y + \partial_y^2 \quad (2)$$

The invariant measure is $\mu = e^{-U(x)} dx \otimes e^{-\frac{y^2}{2}} dy$ so that

$$\partial_x^* = U' - \partial_x, \quad \partial_y^* = y - \partial_y.$$

From now on we will make some assumptions on the potential U :

Assumption 1. *The potential U is smooth, U'' is bounded and $\mu_1 = e^{-U(x)} dx$ satisfies a Poincaré inequality with constant c_U*

We can decompose $L = K + R - R^*$ with

$$\begin{aligned} K &= -\partial_y^* \partial_y \\ R &= -\partial_x^* \partial_y \\ R^* &= -\partial_y^* \partial_x. \end{aligned}$$

We compute in appendix the brackets appearing in Lemma 1 :

Lemma 3.

$$\begin{aligned} [K, R] &= R \\ [K^2, R] &= R(1 + 2K) \\ [R, R^*] &= U'' K + \partial_x^* \partial_x. \end{aligned}$$

As expected the operator $-\partial_x^* \partial_x$ appears in the third derivative:

$$F_t''' = \langle (2K)^3 f_t, f_t \rangle + 12 \langle R(1+2K) f_t, f_t \rangle - 4 \langle \partial_x f_t, \partial_x f_t \rangle + 4 \langle U''(x) \partial_y f_t, \partial_y f_t \rangle .$$

It brings the coercivity in position, which is missing in F_t' . However it is known (cf. [22], [34]) that no linear combination of F_t, F_t', F_t'' and F_t''' can be non-positive for every $f \in L^2(\mu)$. In the particular cases treated in [22] and [34], G_t the norm of the gradient in space appears naturally, thanks to Lemma 2. Indeed the smaller eigenvalue of $\partial_y^* \partial_y$ on $V^\perp = (\text{Ker} \partial_y^* \partial_y)^\perp$ is 1 (Poincaré inequality for the gaussian distribution) and thus

$$\begin{aligned} F_t' &= 2 \langle K f_t, f_t \rangle \\ &= -2 \|\partial_y f_\perp\|^2 \\ &\leq -2 \|f_\perp\|^2 . \end{aligned}$$

In the other hand, Assumption 1 and Lemma 2 ensure $G_t \geq c_U \|f_V\|^2$ and lead to

$$\frac{1}{F_t} \left(G_t - \frac{c_U}{2} F_t' \right) \geq c_U \quad (6)$$

Finally in order to close the differential inequality we need the first derivative of G_t (see Appendix for the proof):

Lemma 4.

$$G_t' = \langle (-2RR^* + 2RU'') f_t, f_t \rangle + 2G_t .$$

We can now find a linear combination of F_t, G_t and their derivatives which is always non-positive. The terms in $\|f_V\|^2$ will be controlled by F_t''' , the ones in $\|f_\perp\|^2$ by F_t' and G_t' .

Lemma 5. *Let $A \in \mathbb{R}$ and $\beta, k > 0$. Under Assumption 1, there exists $\tau_* \in \mathbb{R}$ such that for all $\tau \geq \tau_*$*

$$Q_3(\partial_t) F_t + Q_1(\partial_t) G_t \leq 0$$

with

$$\begin{aligned} Q_1(X) &= 2\beta \left(X + 2 \left(\frac{1}{\beta} - 1 \right) - \frac{k}{2c_U \beta} \right) \\ Q_3(X) &= X^3 + AX^2 + \tau X + k . \end{aligned}$$

Proof. The above computations (Lemma 1 and 3) allow to write, for any $A \in \mathbb{R}$,

$$\begin{aligned} F_t''' + AF_t'' &= \langle ((2K)^3 + A(2K)^2 + 4[[K, R], R - R^*] + 12[K^2, R] + 4A[K, R]) f_t, f_t \rangle \\ &= \langle ((2K)^3 + A(2K)^2 + 4[R, R^*] + 12R(1+2K) + 4AR) f_t, f_t \rangle \\ &= \langle ((2K)^3 + A(2K)^2 - 4U''K - 4\partial_x^* \partial_x + 4R(3+A+6K)) f_t, f_t \rangle \\ &= \langle ((2K)^3 + A(2K)^2 - 4U''K + 4R(3+A+6K)) f_t, f_t \rangle - 4G_t \end{aligned}$$

The operator $R(6+6(2K)+2A)$ is annoying because, as a quadratic form on $L^2(\mu)$, it is neither non-positive nor non-positive ; we'll give for it a not so subtle upper bound by the Cauchy-Schwarz and $2ab \leq a^2 + b^2$ inequalities with the sum of a term RR^* to be controlled by G_t' and of a term only acting on V^\perp , controlled by F_t' .

More precisely, remark that $R = R\pi_\perp$ and furthermore that π_\perp commutes with the self-adjoint operators Id, K and $U''(x)$ which stabilize V (and so V^\perp too). Thus, for any $\beta > 0$,

$$\begin{aligned} &\langle (4R\pi_\perp(3+A+\beta U''+6K)) f_t, f_t \rangle \\ &= 2 \langle (3+A+\beta U''+6K) f_\perp, (2R^*) f_t \rangle \\ &\leq 4\beta \langle RR^* f_t, f_t \rangle + \frac{1}{\beta} \langle (3+A+\beta U''+6K)^2 f_\perp, f_\perp \rangle . \end{aligned}$$

We obtain, taking into account lemma 4,

$$\begin{aligned}
F_t''' + AF_t'' + 2\beta G_t' + 4(1 - \beta)G_t &= \\
&< ((2K)^3 + A(2K)^2 - 4U''K + 4R(3 + A + 6K) - 4\beta RR^* + 4\beta RU'') f_t, f_t > \\
&= < ((2K)^3 + A(2K)^2 - 4U''K - 4\beta RR^*) f_t, f_t > + < 4R(3 + A + \beta U'' + 6K) f_t, f_t > \\
&\leq < ((2K)^3 + A(2K)^2 - 4U''K + \frac{1}{\beta}(3 + A + \beta U'' + 6K)^2) f_\perp, f_\perp > \\
&= < ((2K)^3 + \left(A + \frac{9}{\beta}\right)(2K)^2 + \left(\frac{18 + 6A}{\beta} + 4U''\right)(2K) + \frac{1}{\beta}(3 + A + \beta U'')^2) f_\perp, f_\perp >.
\end{aligned}$$

Now we want to replace the terms with U'' by something that does not depend on x (under Assumption 1).

$$\begin{aligned}
< U'' K f_t, f_t > &= - \iint U''(x) (\partial_y f_t(x, y))^2 \mu(dx, dy) \\
&\leq < (\min U'') K f_t, f_t >
\end{aligned}$$

and

$$< (3 + A + \beta U'')^2 f_\perp, f_\perp > \leq \|3 + A + \beta U''\|_\infty^2 \|f_\perp\|^2.$$

So by denoting

$$P(X) = X^3 + \left(A + \frac{9}{\beta}\right) X^2 + \left(\frac{18 + 6A}{\beta} + 4 \min U''\right) X + \frac{1}{\beta} \|3 + A + \beta U''\|_\infty^2,$$

the previous computation leads to

$$F_t''' + AF_t'' + 2\beta G_t' + 4(1 - \beta)G_t \leq < P(2K) f_\perp, f_\perp >.$$

The eigenvalues of $2K$ on V^\perp being the $-2n$ for $n \in \mathbb{Z}_+$ (the eigenvectors are the so-called Hermite polynomials), consider any $k \geq 0$ and

$$\tau_k = \max_{n \geq 1} \frac{P(-2n) + k}{2n} \quad (< \infty)$$

so that $P(2K) + 2\tau K + k$ gets to be a non-positive bilinear form on V^\perp for all $\tau \geq \tau_k$, in other words

$$< P(2K) f_\perp, f_\perp > \leq -\tau F_t' - k \|f_\perp\|^2.$$

On the other hand $G_t \geq c_U \|f_V\|^2$ (cf. Lemma 2) so that

$$F_t''' + AF_t'' + 2\beta G_t' + \left(4(1 - \beta) - \frac{k}{c_U}\right) G_t + \tau F_t' + k F_t \leq 0.$$

□

Now it remains to get rid of G_t thanks to (6), and to find a common root for Q_1 and Q_3 in order for inequation (4) to hold.

Theorem 2. *Under assumption 1, there exist $\lambda, \eta > 0$, and $t \mapsto \nu_t \geq \nu_* \in \mathbb{R}$ with $\mathcal{R}e(\eta - \sqrt{-\nu_*}) > 0$ such that*

$$(\partial_t + \lambda) \left[(\partial_t + \eta)^2 + \nu_t \right] F_t \leq 0.$$

Proof. Let $A \in \mathbb{R}$ and $\beta \in (0, 1]$. Let $k \in [0, 4c_U(1 - \beta)]$, so that the root of

$$Q_1(X) = 2\beta \left(X + 2\left(\frac{1}{\beta} - 1\right) - \frac{k}{2c_U\beta} \right)$$

is zero for $k = 4c_U(1 - \beta)$ and negative otherwise. Let τ_k be given by Lemma 5; we choose $\tau \geq \tau_{4c_U(1-\beta)}$ large enough such that for all $k \geq 0$

$$Q_3(X) = X^3 + AX^2 + \tau X + k$$

has only one non-positive root, which behaves continuously with respect to k . This root is zero for $k = 0$. Thus there exists a $k \in [0, 4c_U(1 - \beta)]$ such that Q_1 and Q_3 have a common root. We call this root $-\lambda$. Now Lemma 5 can be rewritten, with some constant $u, v, w \in \mathbb{R}$,

$$\begin{aligned} 0 &\geq (\partial_t + \lambda) (F_t'' + uF_t' + vF_t + wG_t) \\ &= (\partial_t + \lambda) \left(F_t'' + \left(u + w\frac{c_U}{2}\right) F_t' + \left(v + w\left(G_t - \frac{c_U}{2}F_t'\right) \frac{1}{F_t}\right) F_t \right). \end{aligned}$$

Let $\eta = \frac{2u + wc_U}{4}$, $\nu_* = v + wc_U - \eta^2$ and

$$\nu_t = \left(v + w\left(G_t - \frac{c_U}{2}F_t'\right) \frac{1}{F_t} \right) - \eta^2.$$

Inequation (6) exactly means $\nu_t \geq \nu_*$. It remains to show that, for some parameters, $-\lambda$ and $\mathcal{R}e(-\eta \pm \sqrt{-\nu_*})$ are negative. These are the real parts of the roots of

$$Q_3(X) + \frac{c_U}{2}XQ_1(X) + c_UQ_1(X) = X^3 + (A + \beta c_U)X^2 + (\tau + 2c_U - \frac{k}{2})X + 2c_U(1 - \beta).$$

Take $\beta = 1$, $A > -c_U$, τ large enough and $k = 0$. Then zero is a common root and

$$Q_3(X) + \frac{c_U}{2}XQ_1(X) + c_UQ_1(X) = X(X^2 + (A + \beta c_U)X + (\tau + 2c_U)),$$

so that $\lambda = 0$. $X^2 + (A + \beta c_U)X + (\tau + 2c_U)$ has positive coefficients so if it has real roots, they are negative. Otherwise $\mathcal{R}e(\eta - \sqrt{-\nu_*}) = \eta = \frac{1}{2}(A + \beta c_U) > 0$. Now if β is chosen slightly less than 1 and k is such that Q_1 and Q_3 still have a common root, relying again on continuity, we still have $\mathcal{R}e(\eta - \sqrt{-\nu_*}) > 0$ but $-\lambda$ becomes a real root of a polynomial with positive coefficient and thus is negative. \square

2.2 The telegraph process

This section is a replica of the previous one. From Lemma 6 to Theorem 3, the generator is

$$Lf(x, y) = y\partial_x(x, y) + a(x, y)(f(x, -y) - f(x, y)). \quad (3)$$

As in the kFP case we compute the derivatives of F_t and G_t , proceed with a differential equation and conclude with a particular choice of the parameters which are in parties to the above approach. First, the invariant measure has to be explicited:

Lemma 6. *The unique (up to a constant) invariant measure of the telegraph model is*

$$\mu = e^{-U(x)} dx \otimes \frac{1}{2} (\delta_1 + \delta_{-1})(dy),$$

where

$$U'(x) = a(x, 1) - a(x, -1).$$

Proof. Note that $yU'(x) = a(x, y) - a(x, -y)$. We check

$$\begin{aligned}\mu Lf &= \iint y \partial_x f(x, y) e^{-U(x)} dx dy + \iint a(x, y) (f(x, -y) - f(x, y)) e^{-U(x)} dx dy \\ &= \iint y f(x, y) U'(x) e^{-U(x)} dx dy + \iint (a(x, -y) - a(x, y)) f(x, y) e^{-U(x)} dx dy \\ &= 0\end{aligned}$$

for all smooth $f \in L^2(\mu)$, so that μ is invariant. In the other hand, the process is clearly recurrent, and uniqueness follows. \square

We note $f_-(x, y) = f(x, -y)$ and remark that

$$V = \{f \in L^2(\mu), f_- = f\} \quad V^\perp = \{f \in L^2(\mu), f_- = -f\}$$

and

$$\pi_\perp f = \frac{f - f_-}{2} \quad \pi_V = \frac{f + f_-}{2}.$$

Thus $yV = V^\perp$ and $yV^\perp = V$, and more precisely

$$\pi_\perp y = y \pi_V \quad \pi_V y = y \pi_\perp.$$

Now define

$$\begin{aligned}Kf &= -(a + a_-) \pi_\perp f \\ Rf &= y (\partial_x - U') \pi_\perp f \\ &= -\pi_V y \partial_x^* \pi_\perp f. \\ R^* f &= -\pi_\perp y \partial_x \pi_V f \\ &= -y \partial_x \left(\frac{f + f_-}{2} \right).\end{aligned}$$

Then

$$\begin{aligned}K + R - R^* &= -(a + a_-) \pi_\perp + y (\partial_x - U') \pi_\perp + y \partial_x \pi_V \\ &= (-a - a_- - y U') \pi_\perp + y \partial_x (\pi_V + \pi_\perp) \\ &= -2a \pi_\perp + y \partial_x \\ &= L.\end{aligned}$$

Note that $a + a_-$ and U' do not depend on y and so, seen as self-adjoint operators on $L^2(\mu)$, they commute with π_\perp and π_V . In particular this gives $K^* = K$.

Now thanks to these considerations we can compute the following brackets (see the appendix for details).

Lemma 7.

$$\begin{aligned}[K, R] &= R(a + a_-) \\ [K^2, R] &= -R(a + a_-)^2 \\ [[K, R], R - R^*] &= R^* R(a + a_-) - R(a + a_-) R^* \\ RR^* &= \partial_x^* \partial_x \pi_V \\ R^* R &= \partial_x^* \partial_x \pi_\perp.\end{aligned}$$

From now on we make the following assumptions:

Assumption 2. The rates $a(\cdot, 1)$ and $a(\cdot, -1)$ are positive, smooth, bounded and with bounded derivatives, and

$$a_* := \min_{\mathbb{R}} (a(\cdot, 1) + a(\cdot, -1)) > 0.$$

Furthermore $U(x) = \int_0^x (a(z, 1) - a(z, -1)) dz$ satisfies Assumption 1.

Then, again F_t is controlled by G_t and F_t' . Indeed, Under Assumption 2,

$$\begin{aligned} F_t' &= 2 \langle K f_t, f_t \rangle \\ &= -2 \langle (a + a_-) f_\perp, f_\perp \rangle \\ &\leq -2a_* \|f_\perp\|^2 \end{aligned}$$

and (Lemma 2),

$$G_t = \|\partial_x f\|^2 \geq \|\partial_x f_V\|^2 \geq c_U \|f_V\|^2$$

so that

$$\frac{1}{F_t} \left(G_t - \frac{c_U}{2a_*} F_t' \right) \geq c_U. \quad (7)$$

We will also need the derivative of G_t , computed in the appendix:

Lemma 8.

$$G_t' = \langle 2(RU'' - R^*R(a + a_-)) f_t, f_t \rangle.$$

We are now ready to prove a result similar to Lemma 5

Lemma 9. Under Assumption 2, there exist polynomials \tilde{Q}_1 and \tilde{Q}_3 respectively of first and third order such that

$$\tilde{Q}_3(\partial_t)F_t + \tilde{Q}_1(\partial_t)G_t \leq 0$$

Proof. Lemma 1 and 7 give, for any $A \in \mathbb{R}$,

$$\begin{aligned} F_t''' + AF_t'' &= \\ &< ((2K)^3 + A(2K)^2 + 4R(-3(a + a_-)^2 + A(a + a_-)) + 4R^*R(a + a_-) - 4R(a + a_-)R^*) f_t, f_t \rangle. \end{aligned}$$

We consider any $h \geq 0$ and write

$$\begin{aligned} F_t''' + AF_t'' + 2(1+h)G_t' &= \\ &< ((2K)^3 + A(2K)^2 + 4R(-3(a + a_-)^2 + A(a + a_-) + (1+h)U'') - 4hR^*R(a + a_-) - 4R(a + a_-)R^*) f_t, f_t \rangle \end{aligned}$$

Now for the extra $-4hR^*R(a + a_-)$, for any $\alpha \in (0, 1]$, via the Cauchy-Schwarz inequality,

$$\begin{aligned} &-4h \langle R^*R(a + a_-) f_t, f_t \rangle \\ &= -4h \langle \partial_x(a + a_-) f_\perp, \partial_x f_\perp \rangle \\ &= -4h \langle (a + a_-) \partial_x f_\perp, \partial_x f_\perp \rangle - 4h \langle (\partial_x(a + a_-)) f_\perp, \partial_x f_\perp \rangle \\ &= -4h \langle (a + a_-) \partial_x f_\perp, \partial_x f_\perp \rangle - 4h \langle (a + a_-)^{-\frac{1}{2}} (\partial_x(a + a_-)) f_\perp, (a + a_-)^{\frac{1}{2}} \partial_x f_\perp \rangle \\ &\leq -4ha_*(1 - \alpha) \|\partial_x f_\perp\|^2 + \frac{h}{\alpha} \|(a + a_-)^{-\frac{1}{2}} (\partial_x(a + a_-)) f_\perp\|^2. \end{aligned}$$

Then following again the steps of Lemma 5, for any $\beta > 0$, we bound

$$\begin{aligned} &< 4R(-3(a + a_-)^2 + A(a + a_-) + (1+h)U'') f_t, f_t \rangle \\ &= 2 \langle (-3(a + a_-)^2 + A(a + a_-) + (1+h)U'') (a + a_-)^{-\frac{1}{2}} f_\perp, 2(a + a_-)^{\frac{1}{2}} R^* f_t \rangle \\ &\leq \frac{1}{\beta} \|(-3(a + a_-)^2 + A(a + a_-) + (1+h)U'') (a + a_-)^{-\frac{1}{2}} f_\perp\|^2 + 4\beta \langle R(a + a_-)R^* f_t, f_t \rangle \end{aligned}$$

Gathering all this, and recalling $K = -(a + a_-)\pi_\perp$ we get

$$\begin{aligned} F_t''' + AF_t'' + 2(1+h)G_t' &\leq \\ &< \left(-8(a+a_-)^3 + 4A(a+a_-)^2 + \frac{(-3(a+a_-)^2 + A(a+a_-) + (1+h)U'')^2}{\beta(a+a_-)} \right) f_\perp, f_\perp > \\ &-4ha_*(1-\alpha)\|\partial_x f_\perp\|^2 + \frac{h}{\alpha} \left\| \frac{\partial_x(a+a_-)}{\sqrt{a+a_-}} f_\perp \right\|^2 - 4 < R(a+a_-)(1-\beta)R^* f_t, f_t >. \end{aligned}$$

For the last term, as long as $\beta \leq 1$,

$$\begin{aligned} -4 < R(a+a_-)(1-\beta)R^* f_t, f_t > &= -4 < (a+a_-)(1-\beta)\partial_x f_V, \partial_x f_V > \\ &\leq -4a_*(1-\beta)\|\partial_x f_V\|^2. \end{aligned}$$

Choose $\alpha < 1$, let $k \in [0, 4c_U(1-\beta)]$ and define h_k such that

$$-4h_k(1-\alpha) = -4(1-\beta) + \frac{k}{a_*c_U}.$$

We will note

$$\lambda_k = a_* \frac{2h_k(1-\alpha)}{(1+h_k)}$$

and define the function

$$H = -8(a+a_-)^3 + 4A(a+a_-)^2 + \frac{(-3(a+a_-)^2 + A(a+a_-) + (1+h)U'')^2}{\beta(a+a_-)} + \frac{h_k(\partial_x(a+a_-))^2}{\alpha(a+a_-)},$$

so that everything comes down to

$$F_t''' + AF_t'' + 2(1+h_k)(G_t' + \lambda_k G_t) \leq < H f_\perp, f_\perp > - \frac{k}{c_U} \|\partial_x f_V\|^2.$$

Under Assumption 2, in one hand Lemma 2 gives $\|\partial_x f_V\|^2 \geq c_U \|f_V\|^2$ and, in the other hand H is bounded; so there exists τ_k such that

$$H - \tau_k(a+a_-) + k \leq 0.$$

Thus, for all $\tau \geq \tau_k$,

$$< H f_\perp, f_\perp > \leq -\tau F_t' - k \|f_\perp\|^2.$$

Finally we get

$$F_t''' + AF_t'' + \tau F_t' + k F_t + 2(1+h_k)(G_t' + \lambda_k G_t) \leq 0.$$

□

Here is ended the proof that (4) is satisfied for the telegraph model:

Theorem 3. *Under assumption 1, there exist $\lambda, \eta > 0$, and $t \mapsto \nu_t \geq \nu_* \in \mathbb{R}$ with $\mathcal{R}e(\eta - \sqrt{-\nu_*}) > 0$ such that*

$$(\partial_t + \lambda) \left[(\partial_t + \eta)^2 + \nu_t \right] F_t \leq 0.$$

Proof. We keep the notations used in the proof of Lemma 9; our purpose is to find some parameters for wich

$$\tilde{Q}_1(X) = 2(1+h_k)(X + \lambda_k)$$

and

$$\tilde{Q}_3(X) = X^3 + AX^2 + \tau X + k$$

have a common root. Let $\beta \in (0, 1]$, $\alpha \in (0, 1)$, $A \in \mathbb{R}$ be fixed, we let k evolve in $[0, 4c_U(1 - \beta)]$. The root of \tilde{Q}_1 ,

$$-\lambda_k = -a_* \frac{2(1 - \beta) - \frac{k}{2c_U}}{(1 + h_k)}$$

is zero for $k = 4c_U(1 - \beta)$, else negative. We take $\tau \geq \tau_{4c_U(1-\beta)}$ large enough so that, for any $k \in [0, 4c_U(1 - \beta)]$, \tilde{Q}_3 has a unique non-positive real root, which evolves continuously with respect to k . This real root is zero for $k = 0$ and so there exists a $k \geq 0$ such that \tilde{Q}_3 and \tilde{Q}_1 have a common root. We call $-\lambda$ this root and consider $u, v, w \in \mathbb{R}$ such that

$$\begin{aligned} \tilde{Q}_3(\partial_t)F_t + \tilde{Q}_1(\partial_t)G_t &= (\partial_t + \lambda) (F_t'' + uF_t' + vF_t + wG_t) \\ &= (\partial_t + \lambda) \left(F_t'' + \left(u + w \frac{c_U}{2a_*} \right) F_t' + \left(v + w \left(G_t - \frac{c_U}{2a_*} F_t' \right) \frac{1}{F_t} \right) F_t \right). \end{aligned}$$

Let $\eta = \frac{2u + a_*^{-1}c_U}{4}$, $\nu_* = v + w c_U - \eta^2$ and

$$\nu_t = \left(v + w \left(G_t - \frac{c_U}{2a_*} F_t' \right) \frac{1}{F_t} \right) - \eta^2.$$

(7) exactly gives $\nu_t \geq \nu_*$. It remains to find some parameters for which $-\lambda$ and $\mathcal{R}e(-\eta \pm \sqrt{-\nu_*})$ are negative. These are the real parts of the roots of

$$\tilde{Q}_3(X) + \frac{c_U}{2a_*} X \tilde{Q}_1(X) + c_U \tilde{Q}_1(X).$$

Take $A > -c_U a_*^{-1}$, $\alpha \in (0, 1)$, $\beta = 1$, τ large enough and $k = 0$, then $h_k = \lambda_k = 0$ and zero is a common root. Thus $\tilde{Q}_1(X) = 2X$ and

$$\tilde{Q}_3(X) + \frac{c_U}{2a_*} X \tilde{Q}_1(X) + c_U \tilde{Q}_1(X) = X \left(X^2 + \left(A + \frac{c_U}{a_*} \right) X + \tau + 2c_U \right).$$

If $X^2 + (A + c_U a_*^{-1}) X + \tau + 2c_U$, polynomial with positive coefficients, has real roots, they are negative, and else $\mathcal{R}e(\eta \pm \sqrt{-\nu_*}) = \eta = \frac{1}{2} (A + c_U a_*^{-1}) > 0$. Now if β is slightly less than 1 this is still the case by continuity, but then $-\lambda$ is a real root of a polynomial with positive coefficient so $\lambda > 0$. □

3 Numerical studies

Although Theorem 1 gives “explicit” bounds for the rate of convergence to equilibrium, it is not very easy to handle, as we get a set of polynomials Π depending on several parameters in some set \mathcal{C} , such that the best rate obtained *via* Theorem 1 is

$$r = \max_{A, \beta, k, \tau \in \mathcal{C}} \min \{ -\mathcal{R}e(\alpha), \alpha \text{ root of } \Pi(X) \}$$

Using the notations of Lemma 5 and 9,

$$\Pi(X) = Q_3(X) + c_U \left(\frac{1}{2c_y} X + 1 \right) Q_1(X)$$

for the kFP process, and

$$\Pi(X) = \tilde{Q}_3(X) + c_U \left(\frac{1}{2a_*} X + 1 \right) \tilde{Q}_1(X)$$

for the telegraph one. \mathcal{C} is the set of parameters for which Q_1 and Q_3 have a common root and the inequality is proven, for instance in the kFP model one need

$$0 < \beta < 1, \quad A > c_U, \quad k > 0, \quad \tau \geq \max_{n \geq 1} \frac{P(-2n) + k}{2n}$$

(P defined in lemma 5). Nevertheless we can deal numerically with this and compare the obtained results with the theoretical rates when they are known, namely in the case of a quadratic potential for the kFP process (see [22]) and for the constant jump rate of the telegraph on the torus (see [34]). Obviously, such examples may just be considered as some benchmarks and are not really interesting processes for MCMC algorithm. As a consequence, once we will have seen the numerical rates can be of the right order of magnitude for the kFP model, we won't push this analysis deeper.

First of all, we adapt Lemma 5 in order to allow some changes in the parameters. The same computations lead to

Lemma 10. *Consider the generator*

$$L_{v,b,U} = v (by\partial_x - U'(x)\partial_y) + (\partial_y^2 - by\partial_y),$$

with invariant measure $e^{-U(x)} dx \otimes e^{b\frac{y^2}{2}}$. Under Assumption 1, for any $A, k \in \mathbb{R}$ and $\beta > 0$ there exists $\tau \in \mathbb{R}$ such that

$$Q_3(\partial_t)F_t + Q_1(\partial_t)G_t \leq 0$$

with

$$Q_1(X) = v^2\beta \left(X + 2b\left(\frac{1}{\beta} - 1\right) - \frac{k}{2v^2c_U\beta} \right)$$

$$Q_3(X) = X^3 + AX^2 + \tau X + k$$

$$\tau \geq \max_{n \geq 1} \frac{P(-2bn) + k}{2bn}$$

$$P(X) = X^3 + \left(A + \frac{9b^2}{\beta} \right) X^2 + \left(6b^2 \frac{3b + A}{\beta} + v^2 \min((6b - 4)U'') \right) X + \frac{1}{\beta} (3b^2 + Ab + v^2\beta \|U''\|_\infty)^2.$$

In the other hand,

$$G_t - \frac{c_U}{2b} F'_t \geq c_U F_t$$

In a MCMC algorithm, U would be given while b^{-1} the variance of the invariant speed and v the ratio between the antisymmetric and symmetric parts of the dynamics should be chosen to get the fastest convergence to equilibrium (given the instantaneous randomness injected in the system).

The exact theoretical exponential rate of convergence for $L_{v,b,U}$ with U'' constant is

$$r_{theor} = 1 - \sqrt{\left(1 - \frac{4v^2U''}{b}\right)_+}.$$

Here are some numerical optimal rates given by Lemma 10 (to be compared to the theoretical one, in brackets if it is not 1) for $U'' = 1$ and different values of v and b (see also figure 3):

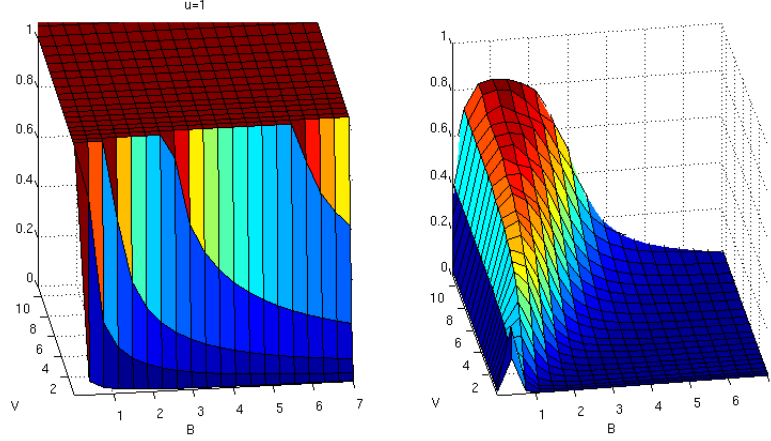


Figure 3: Left: theoretical rate computed in [22]. Right: numerical rate given by Theorem 2. When v is small (*i.e.* the antisymmetric part of L is in a sense weak), the numerical rate is not very accurate and can miss the values for which the non reversible process is faster (asymptotically) than the reversible one. It becomes better with big values of v and for some b we get the right order of magnitude

$v \setminus b$	0.2	0.5	1	3	5
0.5	0.11	0.21	0.02	03.10^{-4} (0.18)	07.10^{-5} (0.10)
1	0.20	0.21	0.07	01.10^{-3}	02.10^{-4} (0.55)
2	0.24	0.26	0.23	06.10^{-3}	01.10^{-3}
10	0.26	0.32	0.56	0.23	0.03

4 Appendix

Proof of Lemma 1:

Proof. From $\partial_t f_t = Lf_t$ comes

$$\begin{aligned} F_t' &= 2 \langle Lf_t, f_t \rangle \\ &= \langle (2K)f_t, f_t \rangle \\ F_t'' &= 2 \langle L^2 f_t, f_t \rangle + 2 \langle Lf_t, Lf_t \rangle \end{aligned}$$

From $(L + L^*)L = 2KL$ we compute

$$\begin{aligned} F_t'' &= \langle (2K)^2 f_t, f_t \rangle + 4 \langle KRf_t, f_t \rangle - 4 \langle KR^* f_t, f_t \rangle \\ &= \langle (2K)^2 f_t, f_t \rangle + 4 \langle [K, R]f_t, f_t \rangle \\ F_t''' &= \langle (2K)^2 Lf_t, f_t \rangle + \langle L^*(2K)^2 f_t, f_t \rangle + 4 \langle [K, R]Lf_t, f_t \rangle + 4 \langle L^*[K, R]f_t, f_t \rangle . \end{aligned}$$

Concerning the first two terms,

$$\begin{aligned} (2K)^2 L + L^*(2K)^2 &= (2K)^3 + (2K)^2(R - R^*) - (R - R^*)(2K)^2 \\ &= (2K)^3 + 4([K^2, R] - [K^2, R^*]) \end{aligned}$$

and $[K^2, R^*]^* = -[K^2, R]$. For the last two terms, $[K, R]K + K[K, R] = [K^2, R]$ thus

$$4 \langle [K, R]Lf_t, f_t \rangle + 4 \langle L^*[K, R]f_t, f_t \rangle = 4 \langle [K^2, R]f_t, f_t \rangle + 4 \langle [[K, R], R - R^*] f_t, f_t \rangle .$$

□

Proof of Lemma 2:

Proof. For the first assertion,

$$\begin{aligned}\int f_V(x)d\mu_1(x) &= \int \left(\int f_t(x, y)d\mu_2(y) \right) d\mu_1(x) \\ &= \mu f_t \\ &= 0.\end{aligned}$$

And so $G_t - \frac{c}{d}F'_t \geq cF_t$ is clear. \square

Proof of Lemma 3:

Proof. First ∂_x and ∂_x^* commute with ∂_y and ∂_y^* , and

$$\begin{aligned}\partial_x \partial_x^* &= \partial_x^* \partial_x + U'' \\ \partial_y \partial_y^* &= \partial_y^* \partial_y + 1.\end{aligned}$$

Now

$$\begin{aligned}[K, R] &= \partial_y^* \partial_y \partial_x^* \partial_y - \partial_x^* \partial_y \partial_y^* \partial_y \\ &= (\partial_y^* \partial_y - \partial_y \partial_y^*) \partial_x^* \partial_y \\ &= R.\end{aligned}$$

As well,

$$\begin{aligned}[K^2, R] &= -(\partial_y^* \partial_y)^2 \partial_x^* \partial_y + \partial_x^* \partial_y (\partial_y^* \partial_y)^2 \\ &= -\partial_x^* (\partial_y \partial_y^* - 1)^2 \partial_y + \partial_x (\partial_y \partial_y^*)^2 \partial_y \\ &= 2\partial_x^* \partial_y \partial_y^* \partial_y - \partial_x^* \partial_y \\ &= R(2K + 1).\end{aligned}$$

Finally

$$\begin{aligned}[R, R^*] &= \partial_x^* \partial_y \partial_y^* \partial_x - \partial_x \partial_y^* \partial_x^* \partial_y \\ &= \partial_x^* \partial_x (\partial_y^* \partial_y + 1) - (\partial_x^* \partial_x + U'') \partial_y^* \partial_y \\ &= -U'' \partial_y^* \partial_y + \partial_x^* \partial_x \\ &= U'' K + \partial_x^* \partial_x.\end{aligned}$$

\square

Proof of Lemma 4:

Proof.

$$\begin{aligned}G'_t &= 2 \langle \partial_x K f_t, \partial_x f_t \rangle + 2 \langle \partial_x (R - R^*) f_t, \partial_x f_t \rangle \\ &= -2 \langle \partial_x^* \partial_x \partial_y^* \partial_y f, f_t \rangle + 2 \langle [\partial_x^* \partial_x, R] f_t, f_t \rangle.\end{aligned}$$

For the first term

$$\begin{aligned}\partial_x^* \partial_x \partial_y^* \partial_y &= \partial_x^* (\partial_y \partial_y^* - 1) \partial_x \\ &= RR^* - \partial_x^* \partial_x,\end{aligned}$$

and for the second one

$$\begin{aligned}\partial_x^* \partial_x R &= -\partial_x^* \partial_x \partial_x^* \partial_y \\ &= -\partial_x^* (\partial_x^* \partial_x + U'') \partial_y \\ &= R \partial_x^* \partial_x + RU''.\end{aligned}$$

Finally,

$$\begin{aligned} G'_t &= \langle (-2RR^* + 2\partial_x^* \partial_x + 2RU'') f_t, f_t \rangle \\ &= \langle (-2RR^* + 2RU'') f_t, f_t \rangle + 2 \langle \partial_x f_t, \partial_x f_t \rangle. \end{aligned}$$

□

Proof of Lemma 7:

Proof.

$$\begin{aligned} [K, R] &= (a + a_-) \pi_\perp \pi_V y \partial_x^* \pi_\perp - \pi_V y \partial_x^* \pi_\perp (a + a_-) \pi_\perp \\ &= 0 + R(a + a_-) \end{aligned}$$

The same computation holds for the second one :

$$\begin{aligned} [K^2, R] &= -((a + a_-) \pi_\perp)^2 \pi_V y \partial_x^* \pi_\perp + \pi_V y \partial_x^* \pi_\perp (a + a_-)^2 \pi_\perp \\ &= 0 - R(a + a_-)^2 \end{aligned}$$

Because $R(a + a_-)R = R^2(a + a_-) = 0$ we have

$$\begin{aligned} [[K, R], R - R^*] &= [R(a + a_-), -R^*] \\ &= R^* R(a + a_-) - R(a + a_-) R^*. \end{aligned}$$

Finally, as $\pi_\perp y \pi_V = y \pi_V$, $\pi_V y \pi_\perp = \pi_V y$ and $y^2 = 1$ we get

$$\begin{aligned} RR^* &= (y \partial_x^* \pi_\perp) (\pi_\perp \partial_x y \pi_V) \\ &= \partial_x^* \partial_x \pi_V \end{aligned}$$

and similarly, as $\pi_\perp y \pi_V = \pi_\perp y$ and $\pi_V y \pi_\perp = y \pi_\perp$,

$$R^* R = \partial_x^* \partial_x \pi_\perp.$$

□

Proof of Lemma 8:

Proof.

$$\begin{aligned} G'_t &= 2 \langle \partial_x^* \partial_x L f_t, f_t \rangle \\ &= 2 \langle \partial_x^* \partial_x R f_t, f_t \rangle - 2 \langle \partial_x^* \partial_x R^* f_t, f_t \rangle - 2 \langle \partial_x^* \partial_x (a + a_-) \pi_\perp f_t, f_t \rangle \\ &= 2 \langle [\partial_x^* \partial_x, R] f_t, f_t \rangle - 2 \langle \partial_x^* \partial_x (a + a_-) \pi_\perp f_t, f_t \rangle. \end{aligned}$$

For the first term,

$$\begin{aligned} [\partial_x^* \partial_x, R] &= -\partial_x^* \partial_x \pi_V y \partial_x^* \pi_\perp + \pi_V y \partial_x^* \pi_\perp \partial_x^* \partial_x \\ &= R[\partial_x, \partial_x^*] \\ &= RU''. \end{aligned}$$

We conclude, according to Lemma 7, with $\partial_x^* \partial_x \pi_\perp = R^* R$.

□

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