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To cite this article: Thierry Bodineau *et al* 2014 *Nonlinearity* **27** 2111

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Lyapunov functionals for boundary-driven nonlinear drift–diffusion equations

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Received 24 July 2013, revised 12 February 2014

Accepted for publication 24 February 2014

Published 1 August 2014

Recommended by C Liverani

Abstract

We exhibit a large class of Lyapunov functionals for nonlinear drift–diffusion equations with non-homogeneous Dirichlet boundary conditions. These are generalizations of large deviation functionals for underlying stochastic many-particle systems, the zero-range process and the Ginzburg–Landau dynamics, which we describe briefly. We prove, as an application, linear inequalities between such an entropy-like functional and its entropy production functional for the boundary-driven porous medium equation in a bounded domain with positive Dirichlet conditions: this implies exponential rates of relaxation related to the first Dirichlet eigenvalue of the domain. We also derive Lyapunov functions for systems of nonlinear diffusion equations, and for nonlinear Markov processes with non-reversible stationary measures.

Keywords: nonlinear diffusion, zero-range process, entropy, entropy, Dirichlet problem

Mathematics Subject Classification: 58J65, 60J60, 60K35, 28D20

1. Introduction

1.1. The setting

We consider a diffusion operator on an open subset Ω in a Riemannian manifold M (Ω may be equal to M): let A be a linear map $T_x M \rightarrow T_x^* M$, $x \in \Omega$. We assume that the associated quadratic form $v \mapsto \langle Av, v \rangle$ is non-negative (on each tangent space), and refer to it as a *diffusion matrix*. We consider a *field* $E : x \in M \rightarrow T_x M$ and define the associated drift-diffusion operator $\mathcal{L} = \mathcal{L}_{A,E}$ by

$$\mathcal{L}_{A,E}\mu := -\nabla^*(A\nabla\mu + E\mu) \quad \text{for } \mu \text{ a measure on } \Omega.$$

Here ∇^* denotes the adjoint operator (i.e. $-\text{div}$ in the case of a flat geometry) and $\nabla\mu$ is defined in the weak sense; if $\mu = h\text{vol}$ then $\nabla\mu = (\nabla h)\text{vol}$ by usual Riemannian calculus (vol is the canonical volume measure on M). We shall always assume that μ has a smooth density, although this assumption can usually be removed by approximation arguments.

We then consider a non-negative function $\sigma : \mathbb{R}_+ \rightarrow \mathbb{R}_+$ that is monotonically increasing on $\mathbb{R}_+$, and a measure ν on Ω . We define the corresponding *nonlinear drift-diffusion equation*

$$\frac{\partial\mu}{\partial t} = \mathcal{L}_{A,E}(\sigma(f)\nu), \quad x \in \Omega, \quad f = \frac{d\mu}{d\nu}. \quad (1.1)$$

In the simplest case where ν is the Lebesgue measure and A the identity, this is just an equation for the density f :

$$\frac{\partial f}{\partial t} = \Delta\sigma(f) + \text{div}(E\sigma(f)).$$

Note that the diffusion coefficient associated with this equation is σ' and is non-negative as σ is assumed to be monotonically increasing. In particular for $\sigma(x) = x^m$, we recover the porous medium equation.

The equation is supplemented with initial conditions and boundary conditions of *non-homogeneous* Dirichlet type:

$$f|_{t=0} = f_0, \quad f|_{\partial\Omega} = f_b \quad (1.2)$$

for some $f_0 \geq 0$ on $x \in \Omega$, and $f_b > 0$ on $x \in \partial\Omega$. This represents an open system in contact at its boundary with reservoirs having specified density values $f_b(x)$ for x in $\partial\Omega$.

Remark 1.1. All our results still hold in the simpler case of *generalized* Neumann boundary conditions (that takes into account the force field E)

$$\forall g \in C_b(\Omega), \quad \int_{\Omega} g \mathcal{L}_{A,E}(\sigma(f)\nu) = \int_{\Omega} \langle A\nabla(\sigma(f)\nu) + E\sigma(f)\nu, \nabla g \rangle, \quad (1.3)$$

that formally is the same as

$$\langle A\nabla(\sigma(f)\nu) + E\sigma(f)\nu, n \rangle = 0 \quad \text{on } \partial\Omega,$$

where $n = n(x)$ is the outward normal to Ω . When $E = 0$, this reduces to the classical Neumann boundary conditions. We also recover previous results in the case of *homogeneous* Dirichlet boundary conditions when f_b is constant.

We finally assume that a stationary measure $d\mu_{\infty} = f_{\infty} d\nu$ exists:

$$\mathcal{L}_{A,E}(\sigma(f_{\infty})\nu) = 0. \quad (1.4)$$

Note that in general the measure $\sigma(f_{\infty})\nu$ is not *reversible*:

$$A\nabla(\sigma(f_{\infty})\nu) + E\sigma(f_{\infty})\nu \neq 0,$$

and f_{∞} is not explicit and depends on the boundary conditions in a non-local manner. This is a manifestation of the open nature of this system.

1.2. The main results

Let us introduce, for any C^2 function $\Phi : \mathbb{R}_+ \rightarrow \mathbb{R}_+$ that satisfies $\Phi(1) = \Phi'(1) = 0$ and $\Phi'' \geq 0$, the following functional:

$$H_\Phi(f|f_\infty) := \int_\Omega \left(\int_{f_\infty(x)}^{f(x)} \Phi' \left(\frac{\sigma(s)}{\sigma(f_\infty(x))} \right) ds \right) dv(x). \quad (1.5)$$

Clearly $\Phi(z) \geq 0$ for $z \in \mathbb{R}_+$ with equality at $z = 1$, and $\Phi'(z) \leq 0$ for $z \in [0, 1]$ and $\Phi'(z) \geq 0$ for $z \in [1, +\infty)$. Due to the fact that σ is monotonically increasing, the functional H_Φ is therefore non-negative.

Remark 1.2. Observe that when $\sigma(s) = s$, this functional reduces to

$$H_\Phi(f|f_\infty) = \int_\Omega \Phi \left(\frac{f}{f_\infty} \right) f_\infty dv = \int_\Omega \Phi \left(\frac{d\mu}{d\mu_\infty} \right) d\mu_\infty.$$

When $\Phi(z) = z \ln z - z + 1$, one recognizes the *Kullback–Leibler information*

$$\int_\Omega d \left(\mu \ln \frac{d\mu}{d\mu_\infty} - \mu + \mu_\infty \right)$$

which differs from Shannon's relative entropy $\int_\Omega d(\mu \ln \frac{d\mu}{d\mu_\infty})$ when μ and μ_∞ have different masses. For lack of a better name, we will use the name '*relative Φ -entropy*' for the functional H_Φ . Note that our definition of entropy has the opposite sign to that used in statistical mechanics or thermodynamics—so it is generally decreasing rather than increasing in time.

Let us also introduce, for any C^2 function $\Psi : \mathbb{R} \rightarrow \mathbb{R}_+$ that satisfies $\Psi'(0) = 0$ and $\Psi'' \geq 0$, the following functional:

$$N_\Psi(f|f_\infty) := \int_\Omega \left(\int_{f_\infty(x)}^{f(x)} \Psi'(\sigma(s) - \sigma(f_\infty(x))) ds \right) dv(x). \quad (1.6)$$

Clearly $\Psi'(z) \geq 0$ for $z \geq 0$ and $\Psi'(z) \leq 0$ for $z \leq 0$. Due to the fact that σ is monotonically increasing, the functional N_Ψ is therefore non-negative again.

Remark 1.3. Observe that when $\sigma(s) = s$, this functional reduces to

$$N_\Psi(f|f_\infty) = \int_\Omega \Psi(f - f_\infty) dv = \int_\Omega \Psi \left(\frac{d\mu}{dv} - \frac{d\mu_\infty}{dv} \right) dv.$$

When $\Psi(z) = z^p$, $p > 1$, one recognizes some kind of Lebesgue norm:

$$\int_\Omega |f - f_\infty|^p dv$$

with respect to the stationary measure. Again for lack of a better name, we will use the name '*relative Ψ -entropy*' for the functional N_Ψ .

Theorem 1.4. Under the previous assumptions, for any solutions $f_t = d\mu_t/dv$ in L^∞ to the nonlinear drift–diffusion equation (1.1)–(1.2), one has in the sense of distribution

$$\frac{d}{dt} H_\Phi(f_t|f_\infty) = - \int_\Omega \Phi''(h) \langle A \nabla h, \nabla h \rangle \sigma(f_\infty) dv \leq 0, \quad h := \frac{\sigma(f)}{\sigma(f_\infty)}.$$

Moreover if v is reversible: $A \nabla v + E v \equiv 0$, then

$$\frac{d}{dt} N_\Psi(f_t|f_\infty) = - \int_\Omega \Psi''(g) \langle A \nabla g, \nabla g \rangle dv \leq 0, \quad g := \sigma(f) - \sigma(f_\infty).$$

Remark 1.5. If $\Phi(z) = z \ln z - z + 1$ and $\sigma(s) = s^m$ then

$$H_\Phi(f|f_\infty) = m \int_\Omega \left(f \ln \frac{f}{f_\infty} - f + f_\infty \right) dv = m \int_\Omega d \left(\mu \ln \frac{d\mu}{d\mu_\infty} - \mu + \mu_\infty \right).$$

(This is independent of the choice of ν .)

If $\Phi(z) = (z - 1)^2/2$ and $\sigma(s) = s^m$, then

$$H_\Phi(f|f_\infty) = \int_\Omega \left(\frac{f^{m+1} - f_\infty^{m+1}}{(m+1)f_\infty^{m+1}} - (f - f_\infty) \right) dv.$$

If $\Psi(z) = z^2/2$, $\sigma(s) = s^m$ and ν is reversible, then

$$N_\Psi(f|f_\infty) = \int_\Omega \left(\frac{f^{m+1} - f_\infty^{m+1}}{(m+1)} - (f - f_\infty)f_\infty^m \right) dv. \quad (1.7)$$

Remark 1.6. As pointed out by an anonymous reviewer, the relative Ψ -entropies introduced above are a natural generalization in the presence of boundary conditions of the entropies discovered and studied by Newman and Ralston in [24, 25] for the porous medium equation in the whole space.

Remark 1.7. Observe that the Φ -entropies and their entropy production functionals measure the distance between f and f_∞ through quotients, whereas the Ψ -entropies and their entropy production functionals measure this distance through differences. Hence one can expect the relation between Φ -entropies and their entropy production functionals to be connected to nonlinear inequalities of logarithmic Sobolev or Beckner type, whereas the relation between Ψ -entropies and their entropy production functionals is connected to *linear* inequalities of Poincaré or spectral theory type.

Our second result is an application of these new entropies to the study of the long-time behaviour of the porous medium equation (PME) in a bounded domain. We assume here that Ω is bounded, $\sigma(s) = s^m$, $m \geq 1$, A is the identity and $\nu = \text{vol}$:

$$\frac{\partial f}{\partial t} = \Delta(f^m) \quad \text{on } \Omega, \quad f|_{t=0} = f_0, \quad f|_{\partial\Omega} = f_b, \quad m \geq 1 \quad (1.8)$$

with $f_0 \geq 0$ on Ω , and $f_b > 0$ and bounded on $\partial\Omega$.

Theorem 1.8. Consider the relative Ψ -entropy (1.7) with $\nu = \text{vol}$; then the solution f_t , $t \geq 0$, to (1.8) in L^∞ satisfies

$$\frac{d}{dt} N_\Psi(f_t|f_\infty) \leq -\lambda N_\Psi(f_t|f_\infty), \quad N_\Psi(f_t|f_\infty) \leq N_\Psi(f_0|f_\infty) e^{-\lambda t}$$

for some constant $\lambda > 0$ depending explicitly on f_b through the bounds on the invariant measure f_∞ and the first Dirichlet eigenvalue of the domain Ω . This implies the convergence $f_t \rightarrow f_\infty$ in time with exponential rate.

1.3. The heuristic for the entropy structure

Our heuristic motivation comes from noting that macroscopic equations of the form (1.1) are meant to describe the coarse-grained evolution of some underlying microscopic system. The time evolution of the macroscopic variables evolving according to (1.1) follows those of the microstates corresponding to almost sure values of the appropriate microscopic functions for the time evolving measure on the microstates. In particular the stationary values of the macrovariables have full measure in the stationary state of the microscopic system. It can then be shown, in cases where (1.1) can be derived from microscopic models, that the large deviation

functionals arising from microscopic dynamics are Lyapunov functions for the macroscopic evolution equation associated with the microscopic dynamics (see [6, 13]). We refer the reader to section 6 for such a derivation in the case where the underlying microscopic model evolves according to a simple stochastic dynamics.

In particular in [6], the relative entropy H_Φ , for $\Phi = z \ln z - z + 1$,

$$H_\Phi(f|f_\infty) := \int_{\Omega} \left(\int_{f_\infty(x)}^{f(x)} \ln \left(\frac{\sigma(s)}{\sigma(f_\infty(x))} \right) ds \right) dx$$

was identified with the large deviation functional of the zero-range process, but the focus was not on the PDE itself, but rather on the stochastic particle system. In (1.5), we generalize this functional to derive a new class of Lyapunov functionals for nonlinear PDE. The functional (1.6) can also be understood as a generalization of the large deviation functional associated with the Ginzburg–Landau process. It is unclear to us whether these functionals are related to the large deviation functionals arising from some other microscopic dynamics. We also refer the reader to [1, 14] where the entropic gradient flow structure is explored on the basis of large deviation principles for linear diffusion equations on the real line (without boundary).

Using such simple models is, heuristically at least, justified by the fact that the macroscopic equations are insensitive to many details of the microscopic dynamics. This is fortunate since the derivation of such macroscopic equations from the true microscopic dynamics, be it Hamiltonian or quantum, is beyond our current mathematical abilities; see [18, 23]. However, even without a rigorous derivation, any macroscopic equation describing the time evolution of a physical system must obviously be consistent with the properties of the microscopic dynamics. Thus, the properly defined macroscopic (Boltzmann) entropy of an isolated system must be monotone. Isolated for equation (1.1) means Neumann or periodic boundary conditions, whereas for the nonlinear Boltzmann equation (appropriate for low density gases) isolated means periodic or specular reflection at the boundary. In both examples the entropy Lyapunov functional is the large deviation functional in the microcanonical ensemble which is stationary for the microscopic dynamics of the isolated system.

The existence of Lyapunov functions for the macroscopic equations can be, and has been, studied independently of any underlying microscopic model. It seems however desirable conceptually and, as we shall see later, in some cases also practically to make the connection between the large deviation functional for the microscopic dynamics and the macroscopic evolution equations. Entropy and large deviation functionals play an important role in the understanding of the macroscopic evolutions in addition to their intrinsic interest for microscopic systems. For references see [18, 23].

1.4. Some references on nonlinear diffusions

The starting point on the study of entropy structure for diffusion equations is arguably the seminal papers of Gross [20] and Bakry and Émery [5], on the logarithmic Sobolev inequality. Then the note [27] exposed the method of Bakry and Émery for proving logarithmic Sobolev inequalities to the kinetic community. The paper [9] used such functional inequalities in order to study the porous medium equation in the whole space (nonlinearity $\sigma(f) = f^m$ with $m > 1$ and $\Omega = \mathbb{R}^d$). Later the paper [10] studied the fast diffusion equation relaxation towards Barenblatt self-similar profiles in the whole space (nonlinearity $\sigma(f) = f^m$ with $(d-2)/2 < m < (d-1)/d$). The paper [8] revisited the whole theory of logarithmic Sobolev and Poincaré inequalities (including the Holley–Stroock criterion for perturbed potentials), for a general class of nonlinearity including fast diffusion and porous medium equations. The paper [4] treats the case of a convex domain with Neumann boundary conditions by a

penalization method (using a limiting process with a ‘barrier’ confining potential). We also refer the reader to [2] for a review of ‘entropy–entropy production methods’ in kinetic theory. Let us also mention the paper [3] providing some refinements of Sobolev inequalities, and the paper [16] which provides a direct proof in the case of Neumann boundary conditions (without penalization), but still with the convexity assumption. Entropy approaches have also been devised for reaction–diffusion-type systems [15].

There is an enormous amount of valuable information in the book of Vazquez [28], centered on the porous medium case ($\sigma(s) = s^m$ with $m > 1$). However, like all previous works it is mainly concerned with the whole space problem, and not so much with entropy structures. The only chapters (19, 20) which are concerned with the asymptotic behaviour of the initial-boundary-value problem are restricted to *homogeneous* Dirichlet boundary conditions in a bounded domain (zero) or in an exterior domain. We also refer the reader to [7] where an entropy was presented for nonlinear diffusions in bounded domains with homogeneous Dirichlet conditions. Hence it seems that there are very few works in the PDE community for the case of a bounded domain with non-homogeneous Dirichlet conditions. This corresponds to f_∞ describing an ‘out-of-equilibrium’ steady solution.

1.5. The plan of the paper

In section 2 we prove theorem 1.4 and in section 3 we prove theorem 1.8. Then section 4 presents an extension of our approach to systems of two nonlinear diffusion equations and derives two Lyapunov functionals in this setting. Section 5 presents an extension to linear or pointwise nonlinear Markov processes with non-reversible stationary measures. Finally in section 6 we explain in detail the heuristic that led us to introduce these relative entropies and entrophies, on the basis of the zero-range process and the Ginzburg–Landau dynamics.

2. Proof of theorem 1.4

Let us first consider the relative Φ -entropy functional H_Φ . The time derivative is

$$\begin{aligned} \frac{d}{dt} H_\Phi(f|f_\infty) &= \int_{\Omega} \Phi' \left(\frac{\sigma(f_t(x))}{\sigma(f_\infty(x))} \right) \frac{d\mathcal{L}_{A,E}(\sigma(f)v)}{dv} dv \\ &= - \int_{\Omega} \Phi' \left(\frac{\sigma(f_t(x))}{\sigma(f_\infty(x))} \right) \nabla^* (A \nabla(\sigma(f)v) + E \sigma(f)v) \, d\text{vol}. \end{aligned}$$

We set $h = \sigma(f)/\sigma(f_\infty)$ and write (using $\mathcal{L}_{A,E}(\sigma(f_\infty)v) = 0$)

$$\begin{aligned} \nabla^* (A \nabla(\sigma(f)v) + E \sigma(f)v) &= \nabla^* (A \nabla(h \sigma(f_\infty)v) + E h \sigma(f_\infty)v) \\ &= \nabla^* A ((\nabla h) \sigma(f_\infty)v) + \langle A \nabla(\sigma(f_\infty)v) + E \sigma(f_\infty)v, \nabla h \rangle. \end{aligned}$$

Since $h \equiv 1$ at the boundary $\partial\Omega$ and $\Phi(1) = \Phi'(1) = 0$ we obtain

$$\begin{aligned} \frac{d}{dt} H_\Phi(f|f_\infty) &= - \int_{\Omega} \Phi'(h) \nabla^* (A \nabla(h \sigma(f_\infty)v) + E h \sigma(f_\infty)v) \, d\text{vol} \\ &= - \int_{\Omega} \Phi'(h) \nabla^* A ((\nabla h) \sigma(f_\infty)v) \, d\text{vol} \\ &\quad - \int_{\Omega} \Phi'(h) \langle A \nabla(\sigma(f_\infty)v) + E \sigma(f_\infty)v, \nabla h \rangle \, d\text{vol} \\ &= - \int_{\Omega} \Phi''(h) \langle \nabla h, A \nabla h \rangle \sigma(f_\infty) \, dv \end{aligned}$$

$$\begin{aligned}
& - \int_{\Omega} \langle A \nabla(\sigma(f_{\infty})v) + E\sigma(f_{\infty})v, \nabla \Phi(h) \rangle \, \mathrm{dvol} \\
& = - \int_{\Omega} \Phi''(h) \langle \nabla h, A \nabla h \rangle \sigma(f_{\infty}) \, \mathrm{d}v \\
& \quad - \int_{\Omega} \Phi(h) \nabla^* (A \nabla(\sigma(f_{\infty})v) + E\sigma(f_{\infty})v) \, \mathrm{dvol} \\
& = - \int_{\Omega} \Phi''(h) \langle \nabla h, A \nabla h \rangle \sigma(f_{\infty}) \, \mathrm{d}v
\end{aligned}$$

which concludes the proof (we have used $\mathcal{L}_{A,E}(\sigma(f_{\infty})v) = 0$ in the two last lines).

Let us next consider the relative Ψ -entropy functional N_{Ψ} . Its time derivative is

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t} N_{\Psi}(f|f_{\infty}) &= \int_{\Omega} \Psi'(\sigma(f_t(x)) - \sigma(f_{\infty}(x))) \frac{\mathrm{d}\mathcal{L}_{A,E}(\sigma(f)v)}{\mathrm{d}v} \, \mathrm{d}v \\
&= - \int_{\Omega} \Psi'(\sigma(f_t(x)) - \sigma(f_{\infty}(x))) \\
&\quad \nabla^* (A \nabla(\sigma(f)v - \sigma(f_{\infty})v) + E(\sigma(f)v - \sigma(f_{\infty})v)) \, \mathrm{dvol}
\end{aligned}$$

where we have again used $\mathcal{L}_{A,E}(\sigma(f_{\infty})v) = 0$ in the last line.

We define $g = \sigma(f) - \sigma(f_{\infty})$ and since $g \equiv 0$ at the boundary $\partial\Omega$ and $\Psi'(0) = 0$ we obtain

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t} N_{\Psi}(f|f_{\infty}) &= - \int_{\Omega} \Psi'(g) \nabla^* (A \nabla(gv) + Egv) \, \mathrm{dvol} \\
&= - \int_{\Omega} \Psi''(g) \langle \nabla g, A \nabla g \rangle \, \mathrm{d}v - \int_{\Omega} \Psi'(g) \nabla^* (g(A \nabla v + Ev)) \, \mathrm{dvol} \\
&= - \int_{\Omega} \Psi''(g) \langle \nabla g, A \nabla g \rangle \, \mathrm{d}v
\end{aligned}$$

which concludes the proof (we have used the reversibility of v in the two last lines).

3. Proof of theorem 1.8

We consider the porous medium equation (1.8) on $\Omega \subset \mathbb{R}^d$ for $\sigma(s) = s^m$, $m \geq 1$ and $v = \mathrm{vol} = \mathrm{d}x$, and the relative Ψ -entropy as constructed before with the choice $\Psi(z) = z^2/2$ (the measure v is reversible and theorem 1.4 applies). This results in

$$\begin{aligned}
N_{\Psi}(f|f_{\infty}) &= \int_{\Omega} \left(\int_{f_{\infty}}^f \Psi'(s^m - f_{\infty}^m) \, \mathrm{d}s \right) \, \mathrm{d}x \\
&= \int_{\Omega} \left(\int_{f_{\infty}}^f (s^m - f_{\infty}^m) \, \mathrm{d}s \right) \, \mathrm{d}x \\
&= \int_{\Omega} \left(\frac{f^{m+1} - f_{\infty}^{m+1}}{m+1} - (f - f_{\infty})f_{\infty}^m \right) \, \mathrm{d}x.
\end{aligned}$$

We have from the previous analysis

$$\frac{\mathrm{d}}{\mathrm{d}t} N_{\Psi}(f_t|f_{\infty}) = - \int_{\Omega} |\nabla(f_t^m - f_{\infty}^m)|^2 \, \mathrm{d}x.$$

We then observe that

$$\int_{\Omega} |\nabla g|^2 \, \mathrm{d}x \geq \lambda_D \int_{\Omega} |g|^2 \, \mathrm{d}x \tag{3.1}$$

for any $g \in H_0^2(\Omega)$ (the Sobolev space with zero boundary conditions $g|_{\partial\Omega} = 0$), where $\lambda_D > 0$ is the first Dirichlet eigenvalue of Ω . We apply this inequality with $g = f^m - f_\infty^m$.

Finally we perform the following elementary calculation in $\mathbb{R}$: for any $y_\infty \in K \subset (0, +\infty)$ with K compact, there is a constant C_K such that

$$\forall y \in \mathbb{R}_+, \quad (y^m - y_\infty^m)^2 \geq C_K \left(\frac{y^{m+1} - y_\infty^{m+1}}{m+1} - (y - y_\infty)y_\infty^m \right)$$

(recall that $m \geq 1$). This inequality is proved as follows. Let $x = y/y_\infty$; then

$$\forall x \in \mathbb{R}_+, \quad (1 - x^m)^2 \geq \frac{C_K y_\infty^{1-m}}{m+1} [x^{m+1} - (m+1)x + m]$$

by considering the three cases $x \sim +\infty$, $x \sim 1$, and $x \sim 0$, and then taking the worst constant over $y_\infty \in K$.

Since f_∞ is valued in a compact subset of $(0, +\infty)$, we finally deduce

$$\frac{d}{dt} N_\Psi(f_t | f_\infty) \leq -\lambda_D C_K N_\Psi(f_t | f_\infty) =: -\lambda N_\Psi(f_t | f_\infty)$$

which concludes the proof.

Remarks 3.1.

- (1) The key ingredient of this proof is equation (3.1). The existence of the positive constant λ_D captures the boundary-driven geometry of the problem through classical *linear* spectral theories for self-adjoint operators with compact resolvent.
- (2) The underlying gradient flow structure shows a typical *hypocoercive* pattern, combining the sum of a partially coercive ‘symmetric’ term and a skew-symmetric non-coercive term. The understanding of this structure is an interesting open question which will be studied in future works.
- (3) Another interesting question is the following. In order to capture the role played by the boundary in a functional inequality, we have used our general framework of Ψ -entropy in order to select an entropy producing an entropy production functional lending itself to a *linear* study. However one could wonder whether this analysis could be performed for the relative Φ -entropy with $\Phi(z) = z \ln z - z + 1$. The key ingredient to be proved would then be a *Dirichlet logarithmic Sobolev inequality*

$$\int_\Omega \frac{|\nabla h|^2}{h} dm \geq \lambda_{\text{DLSI}} \int_\Omega (h \ln h - h + 1) dm$$

for $h \geq 0$ with $h|_{\partial\Omega} = 1$ and m a probability measure on Ω , where $\lambda_{\text{DLSI}} > 0$ depends on μ . By comparison, the usual logarithmic Sobolev inequality only yields

$$\int_\Omega \frac{|\nabla h|^2}{h} dm \geq \lambda_{\text{LSI}} \int_\Omega h \ln \frac{h}{\int_\Omega h dm} dm$$

for some constant $\lambda_{\text{LSI}} > 0$ depending on m . In the latter inequality the integrand involves the non-local quantity $\int_\Omega h dm$ which is non-constant along the flow of the nonlinear diffusion equation. These two inequalities coincide when $\int_\Omega h dm = 1$.

4. The system of nonlinear diffusion equations

In this section, we construct a relative entropy and a relative entropy for a system of two nonlinear equations.

Let $\sigma^1, \sigma^2 : (\mathbb{R}^+)^2 \rightarrow (\mathbb{R}^+)^2$, such that the Jacobian matrix of $(s_1, s_2) \mapsto (\sigma^1(s_1, s_2), \sigma^2(s_1, s_2))$ is definite positive.

We consider two diffusion operators L_{A_1} and L_{A_2} with two diffusion matrices A_1 and A_2 as defined above, and for $\mu(t, x) = (\mu^1(t, x), \mu^2(t, x))^T$ we define the following nonlinear system of diffusion equations:

$$\frac{\partial \mu}{\partial t} = \begin{pmatrix} L_{A_1}(\sigma^1(f)v) \\ L_{A_2}(\sigma^2(f)v) \end{pmatrix}, \quad f = \begin{pmatrix} f^1 \\ f^2 \end{pmatrix} = \begin{pmatrix} d\mu^1/dv \\ d\mu^2/dv \end{pmatrix}, \quad x \in \Omega \quad (4.1)$$

with the initial and boundary conditions

$$f|_{t=0} = f_0 = \begin{pmatrix} f_0^1 \\ f_0^2 \end{pmatrix}, \quad f|_{\partial\Omega} = \begin{pmatrix} f_b^1 \\ f_b^2 \end{pmatrix}$$

for some Borel functions $f_0^1, f_0^2 \geq 0$ on Ω and $f_b^1, f_b^2 > 0$ on $\partial\Omega$, and some reference measure v . We assume the existence of a stationary measure (a solution to this elliptic problem) $(\mu_\infty^1, \mu_\infty^2) = (\sigma^1(f_\infty)v, \sigma^2(f_\infty)v)$, $f_\infty = (f_\infty^1, f_\infty^2)^T$.

We first consider the case of the relative entropy. We assume that the nonlinearity functionals satisfy the compatibility relation

$$\forall s_1, s_2 \in \mathbb{R}_+, \quad \partial_2 \ln \sigma^1(s_1, s_2) = \partial_1 \ln \sigma^2(s_1, s_2), \quad (4.2)$$

where ∂_1, ∂_2 stands for the derivative w.r.t. the first and second coordinates. These relations correspond, in the two-component zero-range process, to a sufficient condition for the stationary microscopic measure to be of the product form; see section 6.

We consider $\Phi(z) = z \ln z - z + 1$ and

$$\begin{aligned} H_\Phi(f|f_\infty) &= \int_\Omega \left(\int_{f_\infty^1}^{f^1} \Phi' \left(\frac{\sigma^1(s, f^2)}{\sigma^1(f_\infty)} \right) ds + \int_{f_\infty^2}^{f^2} \Phi' \left(\frac{\sigma^2(f_\infty^1, s)}{\sigma^2(f_\infty)} \right) ds \right) dv \\ &= \int_\Omega \left(\int_{f_\infty^1}^{f^1} \ln \left(\frac{\sigma^1(s, f^2)}{\sigma^1(f_\infty)} \right) ds + \int_{f_\infty^2}^{f^2} \ln \left(\frac{\sigma^2(f_\infty^1, s)}{\sigma^2(f_\infty)} \right) ds \right) dv. \end{aligned} \quad (4.3)$$

Let us define

$$G_{f_\infty}(f^1, f^2) := \left(\int_{f_\infty^1}^{f^1} \ln \left(\frac{\sigma^1(s, f^2)}{\sigma^1(f_\infty)} \right) ds + \int_{f_\infty^2}^{f^2} \ln \left(\frac{\sigma^2(f_\infty^1, s)}{\sigma^2(f_\infty)} \right) ds \right).$$

Observe that, thanks to the compatibility relation (4.2), one has

$$\begin{aligned} \partial_{f^1} G_{f_\infty}(f^1, f^2) &= \ln \frac{\sigma^1(f)}{\sigma^1(f_\infty)}, \\ \partial_{f^2} G_{f_\infty}(f^1, f^2) &= \ln \frac{\sigma^2(f)}{\sigma^2(f_\infty)}. \end{aligned}$$

Hence we obtain, arguing like for the one-component model,

$$\begin{aligned} \frac{d}{dt} H_\Phi(f_t|f_\infty) &= - \int_\Omega \frac{\langle A_1 \nabla h^1, \nabla h^1 \rangle}{h^1} \sigma^1(f_\infty(x)) dv(x) \\ &\quad - \int_\Omega \frac{\langle A_2 \nabla h^2, \nabla h^2 \rangle}{h^2} \sigma^2(f_\infty(x)) dv(x) \\ &= - \int_\Omega \langle A_1 \nabla \ln h^1, \nabla \ln h^1 \rangle \sigma^1(f(x)) dv(x) \\ &\quad - \int_\Omega \langle A_2 \nabla \ln h^2, \nabla \ln h^2 \rangle \sigma^2(f(x)) dv(x) \leq 0, \end{aligned}$$

where we have used the notation

$$h^1 := \frac{\sigma^1(f)}{\sigma^1(f_\infty)}, \quad h^2 := \frac{\sigma^2(f)}{\sigma^2(f_\infty)}.$$

Remark 4.1. In the case $A_1 = A_2 = \text{Identity}$, the diffusion matrix associated with the evolution is given by

$$\mathbb{D}(s_1, s_2) = \begin{pmatrix} \partial_1 \sigma^1(s_1, s_2) & \partial_2 \sigma^1(s_1, s_2) \\ \partial_1 \sigma^2(s_1, s_2) & \partial_2 \sigma^2(s_1, s_2) \end{pmatrix}$$

and the conductivity matrix is

$$\mathbb{S}(s_1, s_2) = \begin{pmatrix} \sigma^1(s_1, s_2) & 0 \\ 0 & \sigma^2(s_1, s_2) \end{pmatrix}.$$

Then the Hessian matrix of $G_{f_\infty}(s_1, s_2)$ is

$$\mathbb{H}(s_1, s_2) = \begin{pmatrix} \frac{\partial_1 \sigma^1(s_1, s_2)}{\sigma^1(s_1, s_2)} & \frac{\partial_2 \sigma^1(s_1, s_2)}{\sigma^1(s_1, s_2)} \\ \frac{\partial_1 \sigma^2(s_1, s_2)}{\sigma^2(s_1, s_2)} & \frac{\partial_2 \sigma^2(s_1, s_2)}{\sigma^2(s_1, s_2)} \end{pmatrix}$$

and we note that Einstein's relation is satisfied thanks to (4.2):

$$\mathbb{D}(s_1, s_2) = \mathbb{S}(s_1, s_2) \mathbb{H}(s_1, s_2).$$

Remark 4.2. It is natural to ask whether this analysis extends to other relative Φ -entropies, when Φ is different from $\Phi(z) = z \ln z - z + 1$. The compatibility relations (4.2) seem however hard to extend since it is only when $\Phi'(z) = \ln z$ that the 'generalized' condition

$$\partial_2 \Phi' \left(\frac{\sigma^1(s_1, s_2)}{\sigma^1(f_\infty)} \right) = \partial_1 \Phi' \left(\frac{\sigma^2(s_1, s_2)}{\sigma^2(f_\infty)} \right)$$

becomes independent of the values of f_∞ and therefore makes sense.

We next consider the case of the relative entropy. We assume that the nonlinearity functionals satisfy the compatibility relations

$$\forall s_1, s_2 \in \mathbb{R}_+, \quad \partial_2 \sigma^1(s_1, s_2) = \partial_1 \sigma^2(s_1, s_2). \quad (4.4)$$

We consider $\Psi(z) = z^2/2$ and ν reversible, and

$$N_\Psi(f|f_\infty)$$

$$\begin{aligned} &= \int_\Omega \left(\int_{f_\infty^1}^{f^1} \Psi'(\sigma^1(s, f^2) - \sigma^1(f_\infty)) \, ds + \int_{f_\infty^2}^{f^2} \Psi'(\sigma^2(f_\infty^1, s) - \sigma^2(f_\infty)) \, ds \right) d\nu \\ &= \int_\Omega \left(\int_{f_\infty^1}^{f^1} (\sigma^1(s, f^2) - \sigma^1(f_\infty)) \, ds + \int_{f_\infty^2}^{f^2} (\sigma^2(f_\infty^1, s) - \sigma^2(f_\infty)) \, ds \right) d\nu. \end{aligned}$$

Let us define

$$G_{f_\infty}(f^1, f^2) := \left(\int_{f_\infty^1}^{f^1} (\sigma^1(s, f^2) - \sigma^1(f_\infty)) \, ds + \int_{f_\infty^2}^{f^2} (\sigma^2(f_\infty^1, s) - \sigma^2(f_\infty)) \, ds \right).$$

Observe that, thanks to the compatibility relations (4.4), one has

$$\begin{aligned} \partial_{f^1} G_{f_\infty}(f^1, f^2) &= \sigma^1(f) - \sigma^1(f_\infty) \\ \partial_{f^2} G_{f_\infty}(f^1, f^2) &= \sigma^2(f) - \sigma^2(f_\infty). \end{aligned}$$

Hence we obtain, arguing like for the one-component model,

$$\frac{d}{dt} N_\Psi(f_t|f_\infty) = - \int_\Omega \langle A_1 \nabla g^1, g^1 \rangle d\nu(x) - \int_\Omega \langle A_2 \nabla g^2, g^2 \rangle d\nu(x) \leq 0,$$

where we have used the notation

$$g^1 := \sigma^1(f) - \sigma^1(f_\infty), \quad g^2 := \sigma^2(f) - \sigma^2(f_\infty).$$

Remark 4.3. It is again natural to ask whether this analysis extends to other relative Ψ -entropies, when Ψ is different from $\Psi(z) = z^2/2$. The compatibility condition (4.4) seems however hard to extend since it is only when $\Psi'(z) = z$ that the ‘generalized’ condition

$$\partial_2 \Psi'(\sigma^1(x, y) - \sigma^1(f_\infty)) = \partial_1 \Psi'(\sigma^2(x, y) - \sigma^2(f_\infty))$$

becomes independent of the values of f_∞ and therefore makes sense.

Remark 4.4. A simple example of nonlinearity functionals satisfying both compatibility relations is: $\sigma^1(s_1, s_2) = \sigma^2(s_1, s_2) = \varphi(s_1 + s_2)$, for some smooth function φ on $\mathbb{R}_+$. For the particular case $\varphi(z) = z^m$, $m > 0$, one can check that when $\Psi(z) = z^2/2$ and $\nu = \text{vol}$, the relative entropy is

$$N_\Psi(f_t | f_\infty) = \int_\Omega \left(\frac{\Sigma^{m+1} - \Sigma_\infty^{m+1}}{m+1} - (\Sigma - \Sigma_\infty) \Sigma_\infty^m \right) \text{dvol}$$

with $\Sigma = f_t^1 + f_t^2$ and $\Sigma_\infty = f_\infty^1 + f_\infty^2$. When f_∞ is positive and bounded and $m \geq 1$, it is straightforward to prove a linear inequality between the relative entropy and its entropy production in the same manner as in theorem 1.8:

$$\frac{d}{dt} N_\Psi(f_t | f_\infty) \leq -\lambda N_\Psi(f_t | f_\infty)$$

where λ is related to the first Dirichlet eigenvalue of the domain Ω .

5. Nonlinear Markov processes

In this section we consider a measure space $\mathcal{X}$ and a Markov process defined by a kernel $K = K(y, dx)$, which is a measure on $\mathcal{X}$ depending measurably on $y \in \mathcal{X}$. With K there is associated an operator $\mathcal{L} = \mathcal{L}_K$ acting on the space of probability measures on $\mathcal{X}$ defined by

$$\mathcal{L}_K \mu = \int_{y \in \mathcal{X}} K(y, dx) d\mu(y) - \int_{y \in \mathcal{X}} K(x, dy) d\mu(x). \quad (5.1)$$

We assume that there are no problems of integrability, and so all integrals converge, and the Fubini theorem applies whenever needed. In particular,

$$\int_{\mathcal{X}} \mathcal{L}_K \mu = \iint_{\mathcal{X} \times \mathcal{X}} K(y, dx) d\mu(y) - \iint_{\mathcal{X} \times \mathcal{X}} K(x, dy) d\mu(x) = 0. \quad (5.2)$$

A probability measure ν is said to be K -stationary if $\mathcal{L}_K \nu = 0$. It is said to be K -reversible if

$$K(x, dy) d\nu(x) = K(y, dx) d\nu(y).$$

Of course reversibility implies stationarity but the reverse is not true in general. Scattering operators with non-reversible stationary measures can be used for modeling open systems. They resemble nonlinear diffusion with non-homogeneous boundary conditions. In both cases the invariant measure depends in a non-local manner on the global geometry of the problem.

An example is provided by the spatially homogeneous linear Boltzmann equation for the velocity distribution of particles moving among background particles. Letting $(x, y) \rightarrow (v, v')$ denote the velocities after and before collisions, the operator models collisions with background particles for a specified time independent spatially uniform velocity distribution. In the simplest case, the collisions are elastic and the background particles have a Maxwellian distribution with a given temperature. Then the stationary measure is reversible. Another more intricate case is that where the collisions are inelastic and the background particles come off with a non-Maxwellian distribution. The stationary measure is then non-reversible.

Remark 5.1. If $K(y, dx)$ is absolutely continuous with respect to $d\nu(x)$, with density $K(y, x)$, then reversibility for ν means

$$K(x, y) = K(y, x), \quad \nu \otimes \nu\text{-almost surely.}$$

In physical language, this means that the dynamics satisfy detailed balance with respect to the stationary measure ν .

We consider now a nonlinear function $\sigma : \mathbb{R}_+ \rightarrow \mathbb{R}_+$ that is strictly monotonically increasing, and a finite measure ν on $\mathcal{X}$. We define the corresponding *nonlinear scattering equation* describing a nonlinear Markov process:

$$\frac{\partial \mu}{\partial t} = \mathcal{L}_K(\sigma(f)\nu), \quad f := \frac{d\mu}{d\nu} \quad (5.3)$$

complemented with initial conditions $f|_{t=0} = f_0$.

We introduce, similarly to before, for any C^2 function $\Phi : \mathbb{R}_+ \rightarrow \mathbb{R}_+$ that satisfies $\Phi(1) = \Phi'(1) = 0$ and $\Phi'' \geq 0$, the following functional:

$$H_\Phi(f|f_\infty) := \int_{\mathcal{X}} \left(\int_{f_\infty(x)}^{f(x)} \Phi' \left(\frac{\sigma(s)}{\sigma(f_\infty(x))} \right) ds \right) d\nu(x). \quad (5.4)$$

Let us prove:

Proposition 5.2. For any solution $\mu_t = f_t \nu \geq 0$, $f_t \in L^\infty$, to the nonlinear scattering equation (5.3), one has in the sense of distributions

$$\frac{d}{dt} H_\Phi(f_t|f_\infty) = - \iint_{\mathcal{X} \times \mathcal{X}} [(h(y) - h(x))\Phi'(h(y)) + \Phi(h(x)) - \Phi(h(y))]$$

$$K(x, dy)\sigma(f_\infty) d\nu(x) \leq 0,$$

with the notation

$$h := \frac{\sigma(f)}{\sigma(f_\infty)}.$$

Moreover when furthermore ν is K -reversible:

$$K(x, dy) d\nu(x) = K(y, dx) d\nu(y),$$

then N_Ψ , defined in (1.5), satisfies

$$\frac{d}{dt} N_\Psi(f_t|f_\infty)$$

$$= - \int_{\mathcal{X}} [(g(y) - g(x))\Psi'(g(y)) + \Psi(g(x)) - \Psi(g(y))] K(x, dy) d\nu(x) \leq 0$$

with the notation

$$g := \sigma(f) - \sigma(f_\infty).$$

Note that the integrands of the right-hand sides are non-positive due to the convexity of Φ and Ψ .

Proof of proposition 5.2. We first consider the case of the relative Φ -entropy H_Φ . We calculate the time derivative

$$\begin{aligned} \frac{d}{dt} H_\Phi(f_t|f_\infty) &= \int_{\mathcal{X}} \Phi'(h(x)) \mathcal{L}_K(\sigma(f)\nu) = \int_{\mathcal{X}} \Phi'(h(x)) \mathcal{L}_K(h\sigma(f_\infty)\nu) \\ &= \iint_{\mathcal{X} \times \mathcal{X}} \Phi'(h(x)) K(y, dx) h(y) \sigma(f_\infty(y)) d\nu(y) \\ &\quad - \iint_{\mathcal{X} \times \mathcal{X}} \Phi'(h(x)) K(x, dy) h(x) \sigma(f_\infty(x)) d\nu(x) \\ &= \iint_{\mathcal{X} \times \mathcal{X}} h(x) (\Phi'(h(y)) - \Phi'(h(x))) K(x, dy) \sigma(f_\infty(x)) d\nu(x). \end{aligned}$$

Then we use the K -stationarity of $\sigma(f_\infty)\nu$ to deduce

$$\begin{aligned} \iint_{\mathcal{X} \times \mathcal{X}} h(x) \Phi'(h(x)) K(x, dy) \sigma(f_\infty(x)) d\nu(x) \\ = \iint_{\mathcal{X} \times \mathcal{X}} h(y) \Phi'(h(y)) K(x, dy) \sigma(f_\infty(x)) d\nu(x) \end{aligned}$$

and

$$\begin{aligned} \iint_{\mathcal{X} \times \mathcal{X}} \Phi(h(x)) K(x, dy) \sigma(f_\infty(x)) d\nu(x) \\ = \iint_{\mathcal{X} \times \mathcal{X}} \Phi(h(y)) K(x, dy) \sigma(f_\infty(x)) d\nu(x). \end{aligned}$$

This allows us to rewrite the time derivative as

$$\begin{aligned} \frac{d}{dt} H_\Phi(f_t | f_\infty) = - \iint_{\mathcal{X} \times \mathcal{X}} \left[(h(y) - h(x)) \Phi'(h(y)) \right. \\ \left. + \Phi(h(x)) - \Phi(h(y)) \right] K(x, dy) \sigma(f_\infty(x)) d\nu(x) \leq 0 \end{aligned}$$

and concludes the proof.

We next consider the relative Ψ -entropy N_Ψ . Arguing similarly, we calculate

$$\begin{aligned} \frac{d}{dt} N_\Psi(f_t | f_\infty) &= \int_{\mathcal{X}} \Psi'(g(x)) \mathcal{L}_K(\sigma(f)\nu) = \int_{\mathcal{X}} \Psi'(g(x)) \mathcal{L}_K(g\nu) \\ &= \iint_{\mathcal{X} \times \mathcal{X}} \Psi'(g(x)) K(y, dx) g(y) d\nu(y) \\ &\quad - \iint_{\mathcal{X} \times \mathcal{X}} \Psi'(g(x)) K(x, dy) g(x) d\nu(x) \\ &= \iint_{\mathcal{X} \times \mathcal{X}} g(x) (\Psi'(g(y)) - \Psi'(g(x))) K(x, dy) d\nu(x). \end{aligned}$$

Then we use the K -reversibility of ν to deduce

$$\iint_{\mathcal{X} \times \mathcal{X}} g(x) \Psi'(g(x)) K(x, dy) d\nu(x) = \iint_{\mathcal{X} \times \mathcal{X}} g(y) \Psi'(g(y)) K(x, dy) d\nu(x)$$

and

$$\iint_{\mathcal{X} \times \mathcal{X}} \Psi(g(x)) K(x, dy) d\nu(x) = \iint_{\mathcal{X} \times \mathcal{X}} \Psi(g(y)) K(x, dy) d\nu(x).$$

This allows to rewrite the time derivative as

$$\begin{aligned} \frac{d}{dt} N_\Psi(f_t | f_\infty) = - \iint_{\mathcal{X} \times \mathcal{X}} \left[(g(y) - g(x)) \Psi'(g(y)) \right. \\ \left. + \Psi(g(x)) - \Psi(g(y)) \right] K(x, dy) d\nu(x) \leq 0 \end{aligned}$$

and concludes the proof. $\square$

Remark 5.3. In the case of the Φ -entropy H_Φ with $\Phi(z) = z \ln z - z + 1$, an alternative argument is the following: using the exchange of x and y we have

$$\begin{aligned} \frac{d}{dt} H_\Phi(f_t | f_\infty) &= \iint_{\mathcal{X} \times \mathcal{X}} \ln h(x) K(y, dx) h(y) \sigma(f_\infty(y)) dv(y) \\ &\quad - \iint_{\mathcal{X} \times \mathcal{X}} \ln h(x) K(x, dy) h(x) \sigma(f_\infty(x)) dv(x) \\ &= - \iint_{\mathcal{X} \times \mathcal{X}} h(x) \ln \frac{h(x)}{h(y)} K(x, dy) \sigma(f_\infty(x)) dv(x) \\ &= -H(F\pi | G\pi) \leq 0. \end{aligned}$$

Here $H(F\pi | G\pi)$ is the relative entropy between $F\pi$ and $G\pi$ with

$$d\pi(x, y) = K(x, dy) \sigma(f_\infty(x)) dv(x), \quad F(x, y) = h(x), \quad G(x, y) = h(y).$$

By K -stationarity of $\sigma(f_\infty)v$,

$$\begin{aligned} \iint_{\mathcal{X} \times \mathcal{X}} F d\pi(x, y) &= \iint_{\mathcal{X} \times \mathcal{X}} h(x) K(x, dy) \sigma(f_\infty(x)) dv(x) \\ &= \iint_{\mathcal{X} \times \mathcal{X}} h(y) K(x, dy) \sigma(f_\infty(x)) dv(x) = \iint_{\mathcal{X} \times \mathcal{X}} G d\pi(x, y), \end{aligned}$$

and since the measures $F\pi$ and $G\pi$ have same mass, their relative entropy is non-negative.

Remark 5.4. When $\sigma(f_\infty)v$ is K -reversible, there is a simpler proof in the case of the relative Φ -entropy: since $K(x, dy) \sigma(f_\infty(x)) dv(x)$ is invariant under the exchange of x and y , we have

$$\begin{aligned} \frac{d}{dt} H_\Phi(f_t | f_\infty) &= \\ &\quad - \frac{1}{2} \iint_{\mathcal{X} \times \mathcal{X}} [h(x) - h(y)] [\Phi'(h(x)) - \Phi'(h(y))] K(x, dy) \sigma(f_\infty(x)) dv(x) \end{aligned}$$

which is obviously non-positive since $(a - b)(\Phi'(a) - \Phi'(b)) \geq 0$ for all $a, b \geq 0$ due to the convexity of Φ .

6. Microscopic heuristic derivation of relative entropies

In this section, we recall some facts on the zero-range process (ZRP) [17, 26], to provide a heuristic explanation for the Lyapunov function (1.5). The relation between large deviations and Lyapunov functionals has been investigated in [6, 13, 22]. In particular we stress the fact that the Lyapunov function (1.5) was already computed in [6]. We will also recall the definitions of the multi-type zero-range process which is related to the functional (4.3) and of the Ginzburg–Landau dynamics which is associated with the functional (1.6).

6.1. The zero-range process

The ZRP is a lattice gas model with a conservative stochastic dynamics [22] which we define below on the microscopic domain $\Omega_N = \{1, \dots, N\}^d$. The microscopic jump rates of the dynamics are determined by a function $g : \mathbb{N} \rightarrow \mathbb{R}^+$ such that $g(0) = 0$ and, for the sake of simplicity, we assume that g is increasing. In the following, g will be related to the diffusion coefficient σ of the diffusion equation (1.1).

With each site i of Ω_N , one associates an integer variable η_i which specifies the number of particles at this site. The configuration $\eta(t) = \{\eta_i(t)\}_{i \in \Omega_N}$ evolves according to a stochastic

dynamics. Given $\eta(t)$ at time t , a random variable τ_i with exponential rate $N^2 g(\eta_i(t))$ is associated with each site. Let $\tau = \min_i \tau_i$. The configuration remains unchanged until time $t + \tau$; then the site which has the smallest τ_i is updated: a particle at site i jumps randomly to one its neighbors, say j , and the new configuration becomes

$$\eta_i(t + \tau) = \eta_i(t) - 1; \quad \eta_j(t + \tau) = \eta_j(t) + 1; \quad \eta_k(t + \tau) = \eta_k(t), \quad k \neq i, j.$$

Note that if $\eta_i = 0$, then $\tau_i = \infty$ because $g(0) = 0$, and therefore the site cannot be selected. After this update, new variables τ_i are drawn with rates $N^2 g(\eta_i(t + \tau))$ and the same rules apply to the next updates. The case of independent random walks is given by $g(n) = n$: each walk evolves at rate 1 and therefore a site with η_i particles will be updated at rate η_i .

6.2. The invariant measure

The previous dynamics preserve the number of particles and describe an isolated system with an explicit invariant measure. Let m^λ be the probability measure on the integers given by

$$\forall k \in \mathbb{N}^*, \quad m^\lambda(k) = \frac{1}{Z_\lambda} \frac{\lambda^k}{g(1) \cdots g(k)}, \quad (6.1)$$

with $m^\lambda(0) = \frac{1}{Z_\lambda}$ and the normalization constant

$$Z_\lambda = 1 + \sum_{k=1}^{\infty} \frac{\lambda^k}{g(1) \cdots g(k)}.$$

Define $\varphi(\lambda) = \ln Z_\lambda$; then the mean density of particles in the stationary state is obtained as

$$\mathbb{E}_{m^\lambda}(\eta) = \sum_{k=1}^{\infty} k m^\lambda(k) = \lambda \varphi'(\lambda). \quad (6.2)$$

Thus any mean density f can be recovered by tuning λ appropriately: $\lambda = \lambda(f)$, such that $f = \mathbb{E}_{m^\lambda}(\eta)$. In the following, we will index the measure with its mean density f and use the notation $m_f = m^{\lambda(f)}$. We shall see later that the conductivity $\sigma(f)$ at density f can be interpreted as the expectation of g :

$$\sigma(f) = \mathbb{E}_{m_f}(g(\eta)) = \lambda(f). \quad (6.3)$$

The product measure

$$m_{f,N}(\eta) = \bigotimes_{i \in \Omega_N} m_f(\eta_i)$$

is invariant for the ZRP and the measure $m_{f,N}$ conditioned to a fixed number of particles is also invariant (see [26]).

6.3. Static large deviations

Given the mean density $f_\infty \in (0, 1)$, we compute now the large deviations of the measure $m_{f_\infty,N}$. The parameter λ is determined by (6.2) and the relation (6.3) implies that $\sigma(f_\infty) = \lambda$. We will first check that

Lemma 6.1. *The large deviation function of the total density*

$$S_N = \frac{1}{N^d} \sum_{i \in \Omega_N} \eta_i$$

is given by

$$\forall f \in [0, 1], \quad \lim_{\varepsilon \rightarrow 0} \lim_{N \rightarrow \infty} \frac{1}{N^d} \ln \mathbb{P}_{m_{f_\infty, N}}(S_N \in [f - \varepsilon, f + \varepsilon]) = F(f|f_\infty), \quad (6.4)$$

where

$$F(f|f_\infty) := \int_{f_\infty}^f \ln \left(\frac{\sigma(s)}{\sigma(f_\infty)} \right) ds. \quad (6.5)$$

Proof. The large deviation function can be obtained as the Legendre transform of the exponential moments [11]

$$\psi(\gamma) = \lim_{N \rightarrow \infty} \frac{1}{N^d} \ln \mathbb{E}_{m_{f_\infty, N}} \left(\exp(\gamma N^d S_N) \right).$$

As $m_{f_\infty, N}$ is a product measure, the previous expression factorizes and reduces to the computation on one site:

$$\psi(\gamma) = \ln \mathbb{E}_{m_{f_\infty}} \left(\exp(\gamma \eta) \right) = \varphi(\exp(\gamma)\lambda) - \varphi(\lambda). \quad (6.6)$$

The large deviation function $\mathcal{F}(f)$ is the Legendre transform of ψ :

$$\mathcal{F}(f) = \sup_{\gamma} \left\{ \gamma f - [\varphi(\exp(\gamma)\lambda) - \varphi(\lambda)] \right\}. \quad (6.7)$$

The supremum is reached for γ^* such that

$$\mathcal{F}'(f) = \gamma^*, \quad f = \exp(\gamma^*)\lambda \quad \varphi'(\exp(\gamma^*)\lambda).$$

The last equality combined with (6.2) and (6.3) implies that $\sigma(f) = \exp(\gamma^*)\lambda$. As $\lambda = \sigma(f_\infty)$, we deduce that

$$\mathcal{F}(f) = \int_{f_\infty}^f \ln \left(\frac{\sigma(s)}{\sigma(f_\infty)} \right) ds = F(f|f_\infty).$$

This completes (6.4). $\square$

Let us discretize the unit cube $\Omega = [0, 1]^d$ in $\mathbb{R}^d$ with a mesh $1/N$ and embed Ω_N in Ω . The local density of the microscopic system can be viewed as an approximation of a density function $f(x)$ in Ω . To make this quantitative, let us introduce π , the empirical measure associated with the microscopic configuration $\eta = \{\eta_i\}_i$:

$$\pi = \frac{1}{N^d} \sum_{i \in \Omega_N} \eta_i \delta_{\frac{i}{N}}, \quad (6.8)$$

and we say that η approximates the density profile $f(x)$ if π is close to $f(x) dx$ in the weak topology. By abuse of notation, $\text{dist}(\eta, f)$ stands for the distance (for the weak topology) between π and $f(x) dx$.

The large deviations of the local density are given by

Lemma 6.2. *Let f be a smooth density profile in Ω ; then*

$$\lim_{\varepsilon \rightarrow 0} \lim_{N \rightarrow \infty} -\frac{1}{N^d} \ln m_{f_\infty, N}(\{\text{dist}(\eta, f) \leq \varepsilon\}) = \int_{\Omega} F(f(x)|f_\infty) dx. \quad (6.9)$$

As $m_{f_\infty, N}$ is a product measure, the local deviations of the density in a subdomain can be determined by the same computations as in lemma 6.1. The product structure of the measure implies that the costs of the local deviations add up and therefore the large deviation function is the integral of the local costs over the domain.

Observe that the functional in (6.9) is a particular case of the Lyapunov functionals H_Φ introduced in (1.5), when $\Phi(z) = z \ln z - z + 1$, and for Neumann or homogeneous Dirichlet boundary conditions.

6.4. The hydrodynamic limit

We sketch below a heuristic derivation of the hydrodynamic limit for the ZRP and refer the reader to [22] for the proofs.

One chooses the initial data such that the microscopic configuration approximates a smooth macroscopic density profile $f_0(x)$ with $x \in \Omega$. For example, the initial data can be sampled from the product measure

$$m_{f_0, N}(\eta) = \bigotimes_{i \in \Omega_N} m_{f_0(\frac{i}{N})}(\eta_i). \quad (6.10)$$

As f_0 is not constant, this measure is not invariant for the dynamics and the evolution of the local density can be recorded by $\mathbb{E}_{m_{f_0, N}}(\eta_i(t))$. The microscopic evolution rules lead to

$$\partial_t \mathbb{E}_{m_{f_0, N}}(\eta_i(t)) = \frac{N^2}{2d} \sum_{j \sim i} \mathbb{E}_{m_{f_0, N}}(\mathbf{g}(\eta_j(t))) - \mathbb{E}_{m_{f_0, N}}(\mathbf{g}(\eta_i(t))), \quad (6.11)$$

where the sum is over the sites j which are neighbors to i . If $\mathbf{g}$ is not linear, the above equations are not closed and cannot be solved exactly. However, the dynamics equilibrate very fast locally and the density is the only slow mode. Thus one expects, for $i \approx Nx$, local density $f(x, t)$ to be the only relevant parameter and

$$\partial_t f(x, t) = \partial_t \mathbb{E}_{m_{f_0, N}}(\eta_i(t)), \quad \sigma(f(x, t)) = \mathbb{E}_{m_{f_0, N}}(\mathbf{g}(\eta_i(t))),$$

where the conductivity σ is introduced in (6.3). The microscopic equations (6.11) can be understood as a discrete Laplacian which approximates the macroscopic equation

$$\partial_t f(x, t) = \Delta \sigma(f(x, t)). \quad (6.12)$$

Note that the microscopic density, given by $f(i/N, t)$, is slowly varying, so the discrete Laplacian in (6.11) is of order $1/N^2$ which is exactly compensated by the extra factor N^2 of the microscopic jump rates. We remark that the rigorous derivation [22] of (6.12) requires further assumptions on the function $\mathbf{g}$.

In the derivation of (6.12), we have omitted the boundary conditions for simplicity. A more careful computation would lead to Neumann conditions in order to take care of the fact that the particles of the ZRP cannot exit the domain Ω_N .

6.5. Boundary conditions

The hydrodynamic limit (6.12) with Dirichlet boundary conditions can be obtained by taking into account the contribution of reservoirs of particles placed at the boundary of the domain. This is achieved at the microscopic level by introducing new exponential random variables $\{T_i\}$ with rates $N^2 \gamma_i$ for any site i at the boundary of the domain Ω_N . The microscopic dynamics evolve as described previously with updates according to the times $\{\tau_i\} \cup \{T_i\}$. If an update occurs at a time τ_i for a site i at the boundary, a particle jumps uniformly over the nearest neighbors of i ; if the jump occurs outside Ω_N , the particle is removed. If an update occurs at a time T_i , a particle is added at site i . This mimics the role of reservoirs acting at the boundary and maintaining locally a constant density of particles. For any regular density $f_b(x)$ on the boundary $\partial\Omega$ of the macroscopic domain Ω , the parameters γ_i can be tuned such that the hydrodynamic limit satisfies, at any time $t > 0$,

$$\forall x \in \Omega, \quad \partial_t f(x, t) = \Delta \sigma(f(x, t)); \quad f|_{\partial\Omega} = f_b, \quad (6.13)$$

which is the same as equations (1.1)–(1.2) when $A = \text{Identity}$.

For general boundary conditions f_b , a flux of particles is induced by the reservoirs and the stationary state $f_\infty(x)$ is no longer a constant but satisfies

$$\forall x \in \Omega, \quad \Delta \sigma(f_\infty(x)) = 0; \quad f|_{\partial\Omega} = f_b. \quad (6.14)$$

For general microscopic dynamics maintained out of equilibrium by reservoirs, the stationary measure is unknown as the reversibility of the dynamics is broken. However for the ZRP, it has been found in [6, 12] that the invariant measure is a product measure with a varying density

$$m_{f_\infty, N}(\eta) = \bigotimes_{i \in \Omega_N} m_{f_\infty(i/N)}(\eta_i), \quad (6.15)$$

where f_∞ solves (6.14). Thus the large deviations for this new stationary measure can be obtained as in lemma 6.2:

Lemma 6.3. *Let f be a smooth density profile in Ω ; then*

$$\lim_{\varepsilon \rightarrow 0} \lim_{N \rightarrow \infty} -\frac{1}{N^d} \ln m_{f_\infty, N}(\{\text{dist}(\eta, f) \leq \varepsilon\}) = \int_{\Omega} F(f(x)|f_\infty(x)) dx. \quad (6.16)$$

The functional in (6.16) coincides with the Lyapunov functional H_Φ introduced in (1.5) with $\Phi(z) = z \ln z - z + 1$ for general Dirichlet boundary conditions, when $A = \text{Identity}$ and the domain is an open set of $\mathbb{R}^d$.

6.6. Asymmetric evolution

Hydrodynamic equations with an asymmetry $E(x) = (E^{(1)}(x), \dots, E^{(d)}(x))$, $x \in \Omega$, can be derived by modifying the microscopic dynamics as follows. The field $E(x)$ is chosen to be smooth. With each site i of Ω_N , one associates the slow varying field

$$E_i = (E^{(1)}(i/N), \dots, E^{(d)}(i/N)).$$

We introduce the normalization constants

$$\forall i \in \Omega_N, \quad Z_{i, N} = \sum_{\ell=1}^d \exp\left(\frac{1}{2N} E^{(\ell)}(i/N)\right) + \exp\left(-\frac{1}{2N} E^{(\ell)}(i/N)\right).$$

A particle at site i will jump after a random exponential time with rate $N^2 g(\eta_i(t)) Z_{i, N}$, but the jump is no longer uniform on the neighboring sites. A jump in the direction $\pm \vec{e}_\ell$ occurs with probability

$$\frac{1}{Z_{i, N}} \exp\left(\pm \frac{1}{2N} E^{(\ell)}(i/N)\right).$$

Note that the rates are weakly biased by a factor of order $1/N$.

As a consequence the microscopic evolution, equation (6.11) becomes

$$\begin{aligned} & \partial_t \mathbb{E}_{m_{f_0, N}}(\eta_i(t)) \\ &= N^2 \sum_{\ell=1}^d \sum_{s=\pm 1} \exp\left(-\frac{s}{2N} E^{(\ell)}\left(\frac{i+s\vec{e}_\ell}{N}\right)\right) \mathbb{E}_{m_{f_0, N}}(g(\eta_{i+s\vec{e}_\ell}(t))) \\ & \quad - \exp\left(\frac{s}{2N} E^{(\ell)}\left(\frac{i}{N}\right)\right) \mathbb{E}_{m_{f_0, N}}(g(\eta_i(t))) \\ & \simeq N^2 \sum_{\ell=1}^d \sum_{s=\pm 1} \mathbb{E}_{m_{f_0, N}}(g(\eta_{i+s\vec{e}_\ell}(t))) - \mathbb{E}_{m_{f_0, N}}(g(\eta_i(t))) \\ & \quad + \frac{N}{2} \sum_{\ell=1}^d \left[E^{(\ell)}\left(\frac{i-\vec{e}_\ell}{N}\right) \mathbb{E}_{m_{f_0, N}}(g(\eta_{i-\vec{e}_\ell}(t))) - E^{(\ell)}\left(\frac{i+\vec{e}_\ell}{N}\right) \mathbb{E}_{m_{f_0, N}}(g(\eta_{i+\vec{e}_\ell}(t))) \right], \end{aligned}$$

where the second equality is obtained by expanding the weak asymmetry to first order in $1/N$. In the discrete evolution equation, one can identify discrete derivatives (which have a contribution of order $1/N$) and a discrete Laplacian (which has a contribution of order $1/N^2$). The weak asymmetry has been tuned such that in the limit $N \rightarrow \infty$, one gets as in (6.12)

$$\partial_t f(x, t) = \Delta \sigma(f(x, t)) - \operatorname{div}(E(x) \sigma(f(x, t))).$$

We refer the reader to [22] for a rigorous derivation.

6.7. Multi-species ZRP

In [17] a generalization of the ZRP to two species has been proposed. At each site i , we denote by n_i the number of particles of species A and by m_i the number of particles of species B . The jump rates at site i are now given by $u(n_i, m_i)$ for the species A and $v(n_i, m_i)$ for the species B . The conditions imposed on the rates for the stationary measure to be factorized are

$$\frac{u(n_i, m_i)}{u(n_i, m_i - 1)} = \frac{v(n_i, m_i)}{v(n_i - 1, m_i)}. \quad (6.17)$$

At each site, the counterpart of the stationary measure (6.1) is now given by

$$\forall k, \ell \in \mathbb{N}^*, \quad m^{\lambda, \gamma}(k, \ell) = \frac{1}{Z_{\lambda, \gamma}} \frac{\lambda^k}{u(1, \ell) \cdots u(k, \ell)} \frac{\gamma^\ell}{v(0, 1) \cdots v(0, \ell)},$$

where $Z_{\lambda, \gamma}$ is a normalization factor. The case of k species ($k > 2$) can also be defined under similar assumptions (see [19]).

Following the same heuristics as in section 6.4, one recovers the hydrodynamic equations (4.1) when the diffusion matrices are the identity:

$$\frac{\partial}{\partial t} \begin{pmatrix} f^1 \\ f^2 \end{pmatrix} = \Delta \begin{pmatrix} \sigma^1(f^1, f^2) \\ \sigma^2(f^1, f^2) \end{pmatrix}. \quad (6.18)$$

At the macroscopic level, the constraint (6.17) leads to the condition (4.2) on σ_1, σ_2 and the large deviation functional is given by (4.3) with $\Phi(z) = z \ln z - z + 1$. A rigorous derivation of the hydrodynamic equations (in the asymmetric regime) has been achieved in [19].

6.8. Ginzburg–Landau dynamics

We now describe how the functional (1.6) is related to the large deviation functional associated with the Ginzburg–Landau dynamics. Let $\Omega_N = \{1, N\}$ be the one-dimensional periodic domain and V a strictly convex potential (growing fast enough at infinity). The Ginzburg–Landau dynamics is acting on the continuous variables $\xi = \{\xi_i\}_{i \in \Omega_N} \in \mathbb{R}^{\Omega_N}$:

$$d\xi_i(t) = \sum_{j=i \pm 1} (V'(\xi_j) - V'(\xi_i)) dt + \sqrt{2} (dB_{(i, i+1)}(t) - dB_{(i-1, i)}(t)), \quad (6.19)$$

where the $(B_{(i, i+1)}(t))_{i \in \Lambda}$ denote independent standard Brownian motions associated with each edge. We consider periodic boundary conditions for the moment.

The invariant measures are products and can be encoded via the density f as for the ZRP (see section 6.2):

$$\mu_{f, N}(d\xi) = \bigotimes_{i \in \Omega_N} \mu_f(d\xi_i), \quad \text{with} \quad \mu_f(d\xi) = \frac{1}{Z_{\lambda(f)}} \exp(-V(\xi) + \lambda(f)\xi) d\xi, \quad (6.20)$$

where the Lagrange parameter $\lambda(f)$ is tuned such that the mean density under μ_f is equal to f . Define also as in (6.3)

$$\sigma(f) = \mathbb{E}_{\mu_f}(V'(\xi)) = \lambda(f), \quad (6.21)$$

where the last equality follows by integration by parts. It is shown in [21] that after rescaling, the Ginzburg–Landau dynamics follows the hydrodynamic equation $\partial_t f(x, t) = \Delta \sigma(f(x, t))$ (see (6.12)).

Using considerations similar to those in section 6.3, one can show that the large deviation function for the measure $\mu_{f_\infty, N}$ (6.20) with constant density f_∞ is given by

$$\mathcal{G}(f) = \int_0^1 \left(\int_{f_\infty}^{f(x)} [\sigma(s) - \sigma(f_\infty)] \, ds \right) dx. \quad (6.22)$$

One recognizes the Ψ -entropy (1.6) with $\Psi(x) = x^2/2$.

Finally the Ginzburg–Landau dynamics (6.19) can be modified to take into account boundary terms:

$$d\xi_i(t) = \sum_{j=i\pm 1} (V'(\xi_j) - V'(\xi_i)) \, dt + \sqrt{2} (dB_{(i,i+1)}(t) - dB_{(i-1,i)}(t))$$

for $i \neq 1, N$, and

$$\begin{cases} d\xi_1(t) = (V'(\xi_2) - V'(\xi_1)) \, dt + \sqrt{2} dB_{(1,2)}(t) + (a - V'(\xi_1)) \, dt + dB_0(t), \\ d\xi_N(t) = (V'(\xi_{N-1}) - V'(\xi_N)) \, dt - \sqrt{2} dB_{(N-1,N)}(t) \\ \quad + (b - V'(\xi_1)) \, dt + dB_N(t), \end{cases}$$

where B_0 and B_N are two additional independent Brownian motions acting at the boundaries. The reservoirs impose the chemical potentials a and b at the boundaries.

As for the ZRP in contact with reservoirs, the invariant measure remains a product $\otimes_{i=1}^N \mu^{\lambda_i}$ with a linearly varying chemical potential $\lambda_i = a + (b-a)i/(N+1)$ (note that μ^{λ_i} is the measure (6.20) indexed with the chemical potential instead of the density). For this reason, the large deviation functional (6.22) can be generalized when the invariant density profile is no longer constant.

6.9. Large deviations and Lyapunov functions

In the previous section, we recalled that the ZRP in contact with reservoirs satisfies a diffusion equation (6.13) and its invariant measure obeys a large deviation principle (6.16). We will now show that the large deviation function is a Lyapunov function for the limiting equation of the process. As shown in [13], this statement holds in a very general setting (see also [6] for more analytic arguments). Thus we recall the proof in the case of a general particle system.

Consider a microscopic Markovian dynamics with stationary measure ν_N . As in (6.8), $\text{dist}(f, \eta)$ denotes a distance for the weak topology between a density profile f and the empirical measure associated with η .

We suppose that the microscopic system approximates the solution of a PDE (which is assumed to be unique). We now quantify the convergence to the hydrodynamic limit. For any density profile f , define the conditional measure

$$\nu_{f, \varepsilon, N} = \nu_N \left(\cdot \mid \text{dist}(\eta, f) \leq \varepsilon \right).$$

The initial data will be drawn from the measure $\nu_{f_0, \varepsilon, N}$ for ε small enough and therefore concentrate to f_0 (note that this initial measure differs slightly from the one in (6.10)). For any smooth initial data f_0 , we assume that the microscopic dynamics remain close to the macroscopic profile f_t at any time $t > 0$:

$$\forall \delta > 0, \quad \lim_{\varepsilon \rightarrow 0} \lim_{N \rightarrow \infty} \mathbb{E}_{\nu_{f_0, \varepsilon, N}} (\text{dist}(\eta(t), f_t) \leq \delta) = 1, \quad (6.23)$$

where $\mathbb{E}_{\nu_{f_0, \varepsilon, N}}$ stands for the expectation w.r.t. the dynamics starting from the initial data sampled from $\nu_{f_0, \varepsilon, N}$.

Finally, we assume that ν_N obeys a large deviation principle with functional $\mathcal{G}$:

$$\mathcal{G}(f) = \lim_{\varepsilon \rightarrow 0} \lim_{N \rightarrow \infty} -\frac{1}{N^d} \ln \nu_N(\text{dist}(\eta, f) \leq \varepsilon). \quad (6.24)$$

For the ZRP, the previous assumptions are satisfied with the hydrodynamic limit (6.13) and the large deviation principle (6.16).

Proposition 6.4. *Under assumptions (6.23) and (6.24), the large deviation functional $\mathcal{G}$ is a Lyapunov function*

$$\forall t \geq s, \quad \mathcal{G}(f_s) \geq \mathcal{G}(f_t). \quad (6.25)$$

Proof. Fix $\delta > 0$. For $\varepsilon > 0$ small and N large enough, assumption (6.23) implies that

$$\frac{1}{2} \nu_N(\text{dist}(\eta, f) \leq \varepsilon) \leq \mathbb{E}_{\nu_N}(\{\text{dist}(\eta(0), f) \leq \varepsilon\} \cap \{\text{dist}(\eta(t), f_t) \leq \delta\}).$$

Dropping the constraint on the initial data and using the fact that ν_N is the invariant measure, we have

$$\frac{1}{2} \nu_N(\text{dist}(\eta, f) \leq \varepsilon) \leq \mathbb{E}_{\nu_N}(\{\text{dist}(\eta(t), f_t) \leq \delta\}) = \nu_N(\text{dist}(\eta, f_t) \leq \delta).$$

From the large deviations (6.24), we deduce that

$$\forall t \geq 0, \quad \mathcal{G}(f_0) \geq \mathcal{G}(f_t),$$

by letting ε and δ go to 0. Repeating the argument at later times completes (6.25). $\square$

Acknowledgments

This work started at a meeting of the authors at IHES, where JLL was visiting E Carlen and M Carvalho. CM would also like to thank J Dolbeault for numerous discussions on nonlinear diffusions, and for providing references on this topic. We would also like to thank L Bertini, D Gabrielli and J Lasinio for helpful comments. The work of TB was supported by ANR-2010-BLAN-0108. The work of JLL was supported by NSF grant DMR-1104501 and AFOSR grant FA-9550-10-1-0131. The work of CM was supported by the ERC grant MATKIT.

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