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Functional Analysis

The optimal evolution of the free energy of interacting gases and its applications ☆

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Abstract

We establish an inequality for the relative total – internal, potential and interactive – energy of two arbitrary probability densities, their Wasserstein distance, their barycenters and their generalized relative Fisher information. This inequality leads to many known and powerful geometric inequalities, as well as to a remarkable correspondence between ground state solutions of certain quasilinear (or semi-linear) equations and stationary solutions of (non-linear) Fokker–Planck type equations. It also yields the HWBI inequalities – which extend the HWI inequalities in Otto and Villani [J. Funct. Anal. 173 (2) (2000) 361–400], and in Carrillo et al. [Rev. Math. Iberoamericana (2003)], with the additional 'B' referring to the new barycentric term – from which most known Gaussian inequalities can be derived. ***To cite this article: M. Agueh et al., C. R. Acad. Sci. Paris, Ser. I 337 (2003).***

Résumé

L'évolution de l'énergie totale d'un gaz le long d'un transport optimal et applications. Nous établissons une inégalité reliant l'énergie totale – interne, potentielle et interactive – de deux densités de probabilité, leur distance de Wasserstein, leurs barycentres ainsi que leur entropie relative généralisée. Cette inégalité implique plusieurs des inégalités géométriques classiques, ainsi qu'une correspondence remarquable entre les solutions de certaines équations quasilinéaires (ou semi-linéaires) et les solutions stationnaires d'équations du type Fokker–Planck. On établit aussi des inégalités HWBI – généralisant les inégalités HWI de Otto et Villani [J. Funct. Anal. 173 (2) (2000) 361–400] et de Carrillo et al. [Rev. Math. Iberoamericana (2003)], où le « B » refère au nouveau terme barycentrique – dont découlent plusieurs inégalités gaussiennes classiques. ***Pour citer cet article : M. Agueh et al., C. R. Acad. Sci. Paris, Ser. I 337 (2003).***

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Les récents progrès dans la théorie de Monge–Kantorovich du transport de masse ont conduit à des preuves simples et naturelles d'une variété d'inégalités géométriques (voir [9,11,6]). Dans ce même contexte, nous proposons ici une inégalité générale dont découlent la plupart de ces inégalités. À la base, se trouve un principe de comparaison assez simple dans la théorie d'évolution des gaz, qui compare les énergies – interne, potentielle et interactive – de deux états d'un système, après que l'un soit passé à l'autre selon un transport optimal. L'idée principale est de décrire l'évolution de l'énergie totale (1) d'un système, transporté de façon optimale, d'un état $\rho_0 \in \mathcal{P}_a(\Omega)$ à un autre $\rho_1 \in \mathcal{P}_a(\Omega)$, en tenant compte du coût de transport – distance de Wasserstein – (3), des barycentres $b(\rho_0)$ et $b(\rho_1)$ et de l'entropie généralisée (2). Une fois ce principe établi (Section 1), une variété d'inégalités s'en déduisent, en considérant tout simplement quelques exemples d'énergies admissibles (Section 3).

1. Introduction

Let $F:[0,\infty)\to\mathbb{R}$ be continuous, and V (resp., W)$:\mathbb{R}^n\to\mathbb{R}$ be a confinement (resp., interaction) potential, and let $\Omega\subset\mathbb{R}^n$ be open, bounded and convex. The set of probability densities over Ω is denoted by $\mathcal{P}_a(\Omega)$, and the associated *free energy functional* is defined on $\mathcal{P}_a(\Omega)$ by

$$\mathrm{H}_V^{F,W}(\rho)=\int_{\mathbb{R}^n}\left[F(\rho)+\rho V+\frac{1}{2}(W\star\rho)\rho\right]\mathrm{d}x, \tag{1}$$

which is the sum of the internal energy $\mathrm{H}^F(\rho)=\int_{\mathbb{R}^n}F(\rho)\,\mathrm{d}x$, the potential energy $\mathrm{H}_V(\rho)=\int_{\mathbb{R}^n}\rho V\,\mathrm{d}x$ and the interaction energy $\mathrm{H}^W(\rho)=\frac{1}{2}\int_{\mathbb{R}^n}(W\star\rho)\rho\,\mathrm{d}x$. By *Young function*, we mean any nonnegative, C^1, strictly convex function $c:\mathbb{R}^n\to\mathbb{R}$ such that $c(0)=0$ and $\lim_{|x|\to\infty}\frac{c(x)}{|x|}=\infty$.

For $\rho,\rho_0,\rho_1\in\mathcal{P}_a(\Omega)$, we denote by $\mathrm{H}_V^{F,W}(\rho_0|\rho_1):=\mathrm{H}_V^{F,W}(\rho_0)-\mathrm{H}_V^{F,W}(\rho_1)$ the *relative energy of* ρ_0 *with respect to* ρ_1, by $b(\rho):=\int_{\mathbb{R}^n}x\rho(x)\,\mathrm{d}x$ the *barycenter* of ρ, and by

$$I_{c^*}(\rho|\rho_V):=\int_\Omega \rho\nabla\big(F'(\rho)+V+W\star\rho\big)\cdot\nabla c^\star\big(\nabla\big(F'(\rho)+V+W\star\rho\big)\big)\,\mathrm{d}x, \tag{2}$$

the *generalized relative Fisher information of* ρ *with respect to* ρ_V *measured against* c^* (see [5]), where $\rho_V\in\mathcal{P}_a(\Omega)$ satisfies $\nabla(F'(\rho_V)+V+W\star\rho_V)=0$ a.e. When $c(x)=\frac{|x|^2}{2}$, we denote I_{c^*} by I_2. The *Wasserstein distance* between ρ_0 and ρ_1 is defined by

$$W_2(\rho_0,\rho_1)^2:=\inf\left\{\int_{\mathbb{R}^n}|x-Tx|^2\rho_0(x)\,\mathrm{d}x;\ T_\#\rho_0=\rho_1\right\}, \tag{3}$$

where $T_\#\rho_0=\rho_1$ means that $\rho_1(B)=\rho_0(T^{-1}(B))$ for all Borel sets $B\subset\mathbb{R}^n$. In the sequel, $\operatorname{supp}\rho$ denotes the support of $\rho\in\mathcal{P}_a(\Omega)$, c^* is the Legendre transform of c, that is $c^*(y)=\sup_{x\in\mathbb{R}^n}\{x\cdot y-c(x)\}$, $|\Omega|$ is the Lebesgue measure of $\Omega\subset\mathbb{R}^n$, and $q>1$ stands for the conjugate index of $p>1$, $\frac{1}{p}+\frac{1}{q}=1$.

2. Main inequality

Theorem 2.1. *Let* $\Omega\subset\mathbb{R}^n$ *be open, bounded and convex,* $F:[0,\infty)\to\mathbb{R}$ *be differentiable on* $(0,\infty)$ *with* $F(0)=0$ *and* $x\mapsto x^nF(x^{-n})$ *convex and non-increasing, and let* $P_F(x):=xF'(x)-F(x)$ *be its associated pressure function. Let* $V,W:\mathbb{R}^n\to\mathbb{R}$ *be* C^2*-functions with* W *even,* $D^2V\geqslant\lambda I$ *and* $D^2W\geqslant\nu I$ *where* $\lambda,\nu\in\mathbb{R}$, *and I denotes the identity map. Then, for any Young function $c:\mathbb{R}^n \to \mathbb{R}$, we have for all $\rho_0, \rho_1 \in \mathcal{P}_a(\Omega)$ satisfying* $\operatorname{supp}\rho_0 \subset \Omega$ *and* $P_F(\rho_0) \in W^{1,\infty}(\Omega)$,

$$\mathrm{H}_{V+c}^{F,W}(\rho_0|\rho_1) + \frac{\lambda+\nu}{2} W_2^2(\rho_0,\rho_1) - \frac{\nu}{2}\left|\mathrm{b}(\rho_0) - \mathrm{b}(\rho_1)\right|^2 \leqslant \mathrm{H}_{c+\nabla V\cdot x}^{-nP_F,2x\cdot\nabla W}(\rho_0) + \int_\Omega \rho_0 c^*\bigl(-\nabla\bigl(F'(\rho_0) + V + W \star \rho_0\bigr)\bigr)\,\mathrm{d}x, \tag{4}$$

with equality when $\rho_0 = \rho_1 = \rho_{V+c}$, where the latter satisfies

$$\nabla\bigl(F'(\rho_{V+c}) + V + c + W \star \rho_{V+c}\bigr) = 0 \quad a.e. \tag{5}$$

In particular, if $c(x) = c_\sigma(x) = \frac{1}{2\sigma}|x|^2$ for $\sigma > 0$, then we have the identity:

$$\mathrm{H}_V^{F,W}(\rho_0|\rho_1) + \frac{1}{2}\left(\lambda + \nu - \frac{1}{\sigma}\right) W_2^2(\rho_0,\rho_1) - \frac{\nu}{2}\left|\mathrm{b}(\rho_0) - \mathrm{b}(\rho_1)\right|^2 \leqslant \frac{\sigma}{2} I_2(\rho_0|\rho_V). \tag{6}$$

Proof. The proof of (4) relies on the following *energy inequality* which is essentially a compendium of various observations by many authors, McCann [9], Otto [10], Agueh [1], Carillo, McCann and Villani [4] and Cordero, Gangbo and Houdré [5]: for all $\rho_0, \rho_1 \in \mathcal{P}_a(\Omega)$ with $\operatorname{supp}\rho_0 \subset \Omega$ and $P_F(\rho_0) \in W^{1,\infty}(\Omega)$,

$$\mathrm{H}_V^{F,W}(\rho_0) - \mathrm{H}_V^{F,W}(\rho_1) + \frac{\lambda+\nu}{2} W_2^2(\rho_0,\rho_1) - \frac{\nu}{2}\left|\mathrm{b}(\rho_0) - \mathrm{b}(\rho_1)\right|^2 \leqslant \int_\Omega (x - Tx)\cdot\nabla\bigl(F'(\rho_0) + V + W \star \rho_0\bigr)\rho_0\,\mathrm{d}x. \tag{7}$$

This inequality describes the evolution of a generalized energy functional along optimal transport. For its proof, we refer to [1,5]. Using (7) and an integration by parts in $\int_\Omega \rho_0 \nabla(F'(\rho_0))\cdot x\,\mathrm{d}x = \int_\Omega \nabla(P_F(\rho_0))\cdot x\,\mathrm{d}x$, we have that

$$\mathrm{H}_V^{F,W}(\rho_0) - \mathrm{H}_V^{F,W}(\rho_1) + \frac{\lambda+\nu}{2} W_2^2(\rho_0,\rho_1) - \frac{\nu}{2}\left|\mathrm{b}(\rho_0) - \mathrm{b}(\rho_1)\right|^2 \leqslant \mathrm{H}_{x\cdot\nabla V}^{-nP_F,2x\cdot\nabla W}(\rho_0) - \int_\Omega \rho_0\nabla\bigl(F'(\rho_0) + V + W \star \rho_0\bigr)\cdot T(x)\,\mathrm{d}x. \tag{8}$$

Now, use Young inequality $c(y) + c^*(z) \geqslant \langle y, z\rangle$, to obtain:

$$-\nabla\bigl(F'\bigl(\rho_0(x)\bigr) + V(x) + (W\star\rho_0)(x)\bigr)\cdot T(x) \leqslant c\bigl(T(x)\bigr) + c^\star\bigl(-\nabla\bigl(F'\bigl(\rho_0(x)\bigr) + V(x) + (W\star\rho_0)(x)\bigr)\bigr), \tag{9}$$

and then rewrite $\int_\Omega c(T(x))\rho_0(x)\,\mathrm{d}x$ as $\int_\Omega c(y)\rho_1(y)\,\mathrm{d}y$ to conclude (4). Setting $\rho_0 = \rho_1 := \rho_{V+c}$ in (8), we have that $T = I$ and equality holds in (8). Therefore, equality holds in (4) whenever equality holds in (9), where $T(x) = x$. This occurs when (5) is satisfied.

To prove (6), use (4) with c_σ, $V - c_\sigma$ and $\lambda - \frac{1}{\sigma}$, in place of c, V and λ, then observe that

$$\mathrm{H}_{c_\sigma+\nabla(V-c_\sigma)\cdot x}^{-nP_F,2x\cdot\nabla W} + \int_\Omega \rho_0 c_\sigma^\star\bigl(-\nabla\bigl(F'(\rho_0) + V - c_\sigma + W\star\rho_0\bigr)\bigr)\,\mathrm{d}x = \frac{\sigma}{2} I_2(\rho_0|\rho_V). \qquad \square$$

3. Applications

3.1. The case of non (necessarily) quadratic Young functions

The main inequality (4) combined with a scaling argument of the Young function lead to the following optimal Euclidean p-Log Sobolev inequality for any $p > 1$. This inequality was first established by Beckner [3] for $p = 1$, and by Del Pino and Dolbeault for $1 < p < n$. The case where $p > n$ was also established recently and independently by Gentil [8] who used the Prékopa–Leindler inequality and the Hopf–Lax semi-group associated to the Hamilton–Jacobi equation.

Proposition 3.1 (General optimal Euclidean p-Log Sobolev inequality). *Let $\Omega \subset \mathbb{R}^n$ be open bounded and convex, and c be a Young function with p-homogeneous Legendre transform c^*. Then, for all $\rho \in \mathcal{P}_a(\mathbb{R}^n) \cap W^{1,\infty}(\mathbb{R}^n)$ with* $\operatorname{supp} \rho \subset \Omega$,

$$\int_{\mathbb{R}^n} \rho \ln \rho \, \mathrm{d}x \leqslant \frac{n}{p} \ln\left(\frac{p}{n\, \mathrm{e}^{p-1} \sigma_c^{p/n}} \int_{\mathbb{R}^n} \rho c^\star\left(-\frac{\nabla \rho}{\rho}\right) \mathrm{d}x \right), \tag{10}$$

where $\sigma_c = \int_{\mathbb{R}^n} \mathrm{e}^{-c} \, \mathrm{d}x$, and equality holds in (10) *if $\rho(x) = K_\lambda \mathrm{e}^{-\lambda^q c(x)}$ for some $\lambda > 0$, where $K_\lambda = (\int_{\mathbb{R}^n} \mathrm{e}^{-\lambda^q c(x)} \, \mathrm{d}x)^{-1}$. In particular, if $c(x) = (p-1)|x|^p$ and $\rho = |f|^p$, we have for all $f \in W^{1,p}(\mathbb{R}^n)$ with* $\|f\|_p = 1$,

$$\int_{\mathbb{R}^n} |f|^p \ln\bigl(|f|^p\bigr) \, \mathrm{d}x \leqslant \frac{n}{p} \ln\left(C_p \int_{\mathbb{R}^n} |\nabla f|^p \, \mathrm{d}x \right), \tag{11}$$

where

$$C_p = \left(\frac{p}{n}\right)\left(\frac{p-1}{\mathrm{e}}\right)^{p-1} \pi^{-p/2} \left[\frac{\Gamma(\frac{n}{2}+1)}{\Gamma(\frac{n}{q}+1)} \right]^{p/n}.$$

Proof. Use $F(x) = x \ln x$, $c_\lambda(x) = c(\lambda x)$, $\rho_0 = \rho$, $\rho_1 = \mathrm{e}^{-c} / (\int_{\mathbb{R}^n} \mathrm{e}^{-c} \, \mathrm{d}x)$ and $V = W = 0$ in (4), and the fact that c^* is p-homogeneous, to have that

$$\int_{\mathbb{R}^n} \rho \ln \rho \, \mathrm{d}x \leqslant \frac{1}{\lambda^p} \int_{\mathbb{R}^n} \rho c^\star\left(-\frac{\nabla \rho}{\rho}\right) \mathrm{d}x + n \ln \lambda - n - \ln \sigma_c, \tag{12}$$

then show that the infimum over $\lambda > 0$ in (12) is attained at $\bar{\lambda}_\rho = (\frac{p}{n} \int_{\mathbb{R}^n} \rho c^*(-\frac{\nabla \rho}{\rho}) \, \mathrm{d}x)^{1/p}$.

The main inequality (4) applied when $V = W = 0$, leads to a remarkable duality between ground state solutions of some quasilinear (or semi-linear) PDEs and stationary solutions of (non-linear) Fokker–Planck type equations.

Proposition 3.2. *Assume that Ω and F satisfy the hypothesis in Theorem* 2.1, *and let $\psi : \mathbb{R} \to [0, \infty)$ be differentiable and such that $\psi(0) = 0$ and $|\psi^{1/p}(F' \circ \psi)'| = K$ where $p > 1$, and K is chosen to be* 1 *for simplicity. Then, for any q-homogeneous Young function c,*

$$\sup\left\{ -\int_\Omega F(\rho) + c\rho;\ \rho \in \mathcal{P}_a(\Omega) \right\} \leqslant \inf\left\{ \int_\Omega c^*(-\nabla f) - G_F \circ \psi(f);\ f \in C_0^\infty(\Omega),\ \int_\Omega \psi(f) = 1 \right\}, \tag{13}$$

where $G_F(x) := (1-n)F(x) + nxF'(x)$. Furthermore, equality holds in (13) *if there exists $\bar{f}$ (and $\bar{\rho} = \psi(\bar{f})$) that satisfies the ODE*

$$-(F' \circ \psi)'(\bar{f}) \nabla \bar{f}(x) = \nabla c(x) \quad \text{a.e.} \tag{14}$$

Moreover, $\bar f$ solves the quasilinear PDE

$$\begin{aligned} &\operatorname{div}\{\nabla c^*(-\nabla f)\} - (G_F\circ\psi)'(f) = \lambda\psi'(f) && \text{in } \Omega,\\ &\nabla c^*(-\nabla f)\cdot\nu = 0 && \text{on } \partial\Omega, \end{aligned} \tag{15}$$

for some $\lambda\in\mathbb{R}$, while $\bar\rho$ is a stationary solution of the Fokker–Planck type equation

$$\begin{aligned} &\tfrac{\partial\rho}{\partial t} = \operatorname{div}\{\rho\nabla(F'(\rho)+c)\} && \text{in } (0,\infty)\times\Omega,\\ &\rho\nabla\big(F'(\rho)+c\big)\cdot\nu = 0 && \text{on } (0,\infty)\times\partial\Omega. \end{aligned} \tag{16}$$

Proof. Let $Q''(x) = x^{1/q}F''(x)$,

$$J(\rho) := -\int_\Omega \big(F(\rho)+c\rho\big)\,\mathrm{d}y \quad\text{and}\quad \tilde J(\rho) := -\int_\Omega (F+nP_F)(\rho)\,\mathrm{d}x + \int_\Omega c^*\big(-\nabla\big(Q'(\rho)\big)\big)\,\mathrm{d}x.$$

From Theorem 2.1, $J(\rho)\leqslant \tilde J(\psi(f))$ for all $\rho\in\mathcal{P}_a(\Omega)$ and $f\in C_c^\infty(\Omega)$ with $\int_\Omega\psi(f)\,\mathrm{d}x = 1$, and equality holds for $\bar\rho = \psi(\bar f)$ satisfying (14). This, combined with the assumption $|\psi^{1/p}(F'\circ\psi)'| = 1$ and the q-homogeneity of c^* proves (13). The Euler–Lagrange equation of the right-hand side of (13) is (15), where λ is a Lagrange multiplier. Using the arguments in [10], one sees that the maximizer $\bar\rho$ of the left-hand side of (13) is a stationary solution of (16). □

Proposition 3.2 applied to $F(x) = \frac{x^\gamma}{\gamma-1}$ where $1\neq 1-\frac1n$, and $c(x) = \frac{r\gamma}{2}|x|^2$ where $r\in(0,\frac{2n}{n-2}]$, yields the optimal Sobolev and Gagliardo–Nirenberg inequalities recently obtained in [7] and [6]. (See details in [2].)

Corollary 3.3 (Optimal Sobolev and Gagliardo–Nirenberg inequalities). *Let $1<p<n$ and $r\in(0,p^*)$, with $r\neq p$ and $p^* = \frac{np}{n-p}$. Set $\gamma := \frac1r + \frac1q$, where $\frac1p+\frac1q = 1$. Then, for any $f\in W^{1,p}(\mathbb{R}^n)$, we have the Gagliardo–Nirenberg inequality*:

$$\|f\|_r \leqslant C(p,r)\|\nabla f\|_p^\theta \|f\|_{r\gamma}^{1-\theta}, \tag{17}$$

where $\frac1r = \frac{\theta}{p^*} + \frac{1-\theta}{r\gamma}$, and the best constant $C(p,r)>0$ can be obtained by scaling.

In particular, if $r = p^*$, we have the Sobolev inequality: $\|f\|_r\leqslant C(p,n)\|\nabla f\|_p$, *where the best constant $C(p,n)>0$ can be obtained from* (13) *and* (14).

3.2. The case of quadratic Young functions

Here, we establish the HWBI inequality, an extension of the HWI inequality in [11], and we deduce extensions of generalized Log-Sobolev and Talagrand inequalities recently obtained in [4].

Proposition 3.4 (HWBI inequalities). *Assume that Ω, F, W and V satisfy the hypothesis in Theorem* 2.1. *Then, we have for all $\rho_0,\rho_1\in\mathcal{P}_a(\Omega)$ with $\operatorname{supp}\rho_0\subset\Omega$ and $P_F(\rho_0)\in W^{1,\infty}(\Omega)$,*

$$\mathrm{H}_V^{F,W}(\rho_0|\rho_1) \leqslant W_2(\rho_0,\rho_1)\sqrt{I_2(\rho_0|\rho_V)} - \frac{\lambda+\nu}{2}W_2^2(\rho_0,\rho_1) + \frac{\nu}{2}\big|\mathrm{b}(\rho_0)-\mathrm{b}(\rho_1)\big|^2. \tag{18}$$

Proof. Rewrite (6) as

$$\mathrm{H}_V^{F,W}(\rho_0|\rho_1) + \frac{\lambda+\nu}{2}W_2^2(\rho_0,\rho_1) - \frac{\nu}{2}\big|\mathrm{b}(\rho_0)-\mathrm{b}(\rho_1)\big|^2 \leqslant \frac{1}{2\sigma}W_2^2(\rho_0,\rho_1) + \frac{\sigma}{2}I_2(\rho_0|\rho_V), \tag{19}$$

and show that the minimizer over $\sigma>0$ of (19) is attained at $\bar\sigma = \frac{W_2(\rho_0,\rho_1)}{\sqrt{I_2(\rho_0|\rho_V)}}$.

Corollary 3.5 (Generalized Log-Sobolev and Talagrand inequalities). *In addition to the hypothesis on Ω, F, V, W in Theorem* 2.1, *assume that* $\lambda+\nu>0$. *Then, for all* $\rho, \rho_0, \rho_1 \in \mathcal{P}_a(\Omega)$ *with* $\operatorname{supp}\rho_0 \subset \Omega$ *and* $P_F(\rho_0) \in W^{1,\infty}(\Omega)$, *we have*

$$\mathrm{H}_V^{F,W}(\rho_0|\rho_1) - \frac{\nu}{2}\big|\mathrm{b}(\rho_0)-\mathrm{b}(\rho_1)\big|^2 \leqslant \frac{1}{2(\lambda+\nu)} I_2(\rho_0|\rho_V), \quad \textit{and} \tag{20}$$

$$\frac{\lambda+\nu}{2} W_2^2(\rho,\rho_V) - \frac{\nu}{2}\big|\mathrm{b}(\rho)-\mathrm{b}(\rho_V)\big|^2 \leqslant \mathrm{H}_V^{F,W}(\rho|\rho_V). \tag{21}$$

Furthermore, if W is convex, then

$$\mathrm{H}_V^{F,W}(\rho_0|\rho_1) \leqslant \frac{1}{2\lambda} I_2(\rho_0|\rho_V), \quad \textit{and} \quad W_2(\rho,\rho_V) \leqslant \sqrt{\frac{2\mathrm{H}_V^{F,W}(\rho|\rho_V)}{\lambda}}. \tag{22}$$

Many Gaussian inequalities can be derived from (6), (22) and (22) (see details in [2,11]). Also, using (20)–(22), one can recover results obtained in [4] for the trend to equilibrium of Fokker–Planck and McKean–Vlasov type equations (see details in [2,4]).

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