On constrained optimization in the Wasserstein metric

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Abstract

In this paper we prove the monotonicity of the second-order moments of the discrete approximations to the heat equation arising from the Jordan-Kinderlehrer-Otto (JKO) variational scheme [7]. This issue appears in the study of constrained optimization in the 2-Wasserstein metric performed by Carlen and Gangbo [3] via a duality argument. A direct argument, via Lagrange multipliers, is outlined in [3] and provided here.

1 Introduction

In [3], the authors perform a comprehensive study of constrained optimization in the space of probability densities with finite second-order moments over $\mathbb{R}^N$. An application is provided in [4].

Given a probability density ρ_0 on $\mathbb{R}^N$ with finite second-order moment, one seeks to minimize

$$I[\rho_0;\tau](\rho) := \frac{1}{2\tau} d(\rho,\rho_0)^2 + \int_{\mathbb{R}^N} \rho(x)\log\rho(x)dx, \tag{1.1}$$

over all $\rho \in \mathcal{M}$ having the same mean and variance as ρ_0, where $\tau > 0$ and

$$\mathcal{M} := \left\{ \rho : \mathbb{R}^N \to [0,\infty) \;\middle|\; \int_{\mathbb{R}^N} \rho(x)dx = 1,\ \int_{\mathbb{R}^N} |x|^2\rho(x)dx < +\infty \right\}.$$

More precisely, for given $u \in \mathbb{R}^N$ and $\theta > 0$, if we denote by

$$\mathcal{E}_{\theta,u} := \left\{ \rho \in \mathcal{M} \;\middle|\; \int_{\mathbb{R}^N} x\rho(x)dx = u,\ \int_{\mathbb{R}^N} |x-u|^2\rho(x)dx = \theta \right\} \tag{1.2}$$

and take $\rho_0 \in \mathcal{E}_{\theta,u}$, we wish to prove the existence of a minimizer in $\mathcal{E}_{\theta,u}$ for $I[\rho_0]$ defined in (1.1).

The duality argument used in [3], although natural and enlightening, appears complicated and could readily be replaced, as the authors of [3] observe, by an easier one based on Lagrange multipliers if one knew that the unconstrained minimizer $\rho_1 \in \mathcal{M}$ of $I[\rho_0]$ satisfied

$$\int_{\mathbb{R}^N} |x|^2 \rho_1(x) dx > \int_{\mathbb{R}^N} |x|^2 \rho_0(x) dx, \tag{1.3}$$

i.e. the minimization

$$\inf_{\rho \in \mathcal{M}} I[\rho_0; \tau](\rho) \tag{1.4}$$

increases the second-order moments. The inequality (1.3) is only conjectured in [3]. We are going to prove:

Theorem 1. *For every $\rho_0 \in \mathcal{M}$ and every $\tau > 0$, the minimizer*

$$\rho_1 := \arg\min_{\rho \in \mathcal{M}} I[\rho_0; \tau](\rho)$$

satisfies

$$\int_{\mathbb{R}^N} |x|^2 \rho_1(x) dx \geq N\tau + \int_{\mathbb{R}^N} |x|^2 \rho_0(x) dx. \tag{1.5}$$

The next statement will also be proved.

Proposition 1. *Within the above notation and hypotheses,*

$$\int_{\mathbb{R}^N} |x|^2 \rho_1(x) dx - \int_{\mathbb{R}^N} |x|^2 \rho_0(x) dx = 2N\tau - d(\rho_0, \rho_1)^2. \tag{1.6}$$

We then have:

Corollary 1. *Within the above notation and hypotheses,*

$$d(\rho_0, \rho_1)^2 \leq N\tau. \tag{1.7}$$

2 Regularity of the minimizer

We shall first work under the extra assumption that $\rho_0 \in L^\infty(\mathbb{R}^N)$. Though the general case will not be built on this, most of the arguments will be the same. Our choice of discussing the essentially bounded case separately resides in the discrete comparison principle stated and proved next. Although based on earlier work by different authors [8], [1], [6], [9], there are significant issues arising due to the unboundedness of the domain and the singularity of the logarithmic function at zero. Therefore, we find this result interesting in itself.

2.1 Discrete comparison principle and regularity in the essentially bounded case

We will prove the following:

Proposition 2. *If $\rho_0 \in \mathcal{M} \cap L^\infty(\mathbb{R}^N)$, then the minimizer ρ_1 of (1.4) is also essentially bounded in $\mathbb{R}^N$ and satisfies*

$$\|\rho_1\|_\infty \le \|\rho_0\|_\infty.$$

Proof: Let $\phi(z) = z\log z$ and let $M \ge \|\rho_0\|_\infty$ be fixed. Take $\mu \in P(\rho_0, \rho_1)$ to be the optimal transfer plan, and let $E := \{\rho_1 > M\}$ assuming $|E| > 0$. Then $\mu((\mathbb{R}^N \backslash E) \times E) > 0$. Otherwise

$$M|E| < \int_E \rho_1 dx = \mu(\mathbb{R}^N \times E) = \mu(E \times E) \le \mu(E \times \mathbb{R}^N) = \int_E \rho_0 dx \le M|E|,$$

which is a contradiction. Now define w_0 and w_1 by

$$\int_{\mathbb{R}^N} w_0 \xi dx = \iint_{(\mathbb{R}^N \backslash E)\times E} \xi(x) d\mu(x,y),$$

$$\int_{\mathbb{R}^N} w_1 \xi dx = \iint_{(\mathbb{R}^N \backslash E)\times E} \xi(y) d\mu(x,y),$$

for all $\xi \in C(\mathbb{R}^N)$. It is easy to check that $0 \le w_0 \le \rho_0 \le M$ and $0 \le w_1 \le \rho_1$. Then, the equality (valid for all $\xi \in C(\mathbb{R}^N \times \mathbb{R}^N)$)

$$\iint_{\mathbb{R}^N\times\mathbb{R}^N} \xi(x,y) d\mu_s(x,y) = \iint_{\mathbb{R}^N\times\mathbb{R}^N} \xi(x,y) d\mu(x,y) + s \iint_{(\mathbb{R}^N \backslash E)\times E} \big(\xi(x,x) - \xi(x,y)\big) d\mu(x,y),$$

defines for every $s \ll 1$ a plan $\mu_s \in P(\rho_0, \rho_s)$ with $\rho_s := \rho_1 - s(w_1 - w_0) \in \mathcal{M}$. Then

$$\begin{aligned} &\frac{1}{2\tau} d(\rho_0, \rho_s)^2 + \int_{\mathbb{R}^N} \phi(\rho_s) dx \qquad (2.1)\\ &\qquad \le I[\rho_0; \tau](\rho_1) + \int_{\mathbb{R}^N} [\phi(\rho_s) - \phi(\rho_1)] dx - \frac{s}{2\tau} \iint_{(\mathbb{R}^N \backslash E)\times E} |x-y|^2 d\mu(x,y) \end{aligned}$$

due to the definition of d and μ_s. Due to the convexity of ϕ and the fact that w integrates to 0, we have

$$\begin{aligned} \int_{\mathbb{R}^N} [\phi(\rho_s) - \phi(\rho_1)] dx &\le \int_{\mathbb{R}^N} (\rho_s - \rho_1) \log \rho_s dx \\ &= -s \int_{\mathbb{R}^N} [\log \rho_s - \log M] w dx \end{aligned}$$

$$= -s \int_E [\log(\rho_1 - s w_1) - \log M] w_1 dx + s \int_{\mathbb{R}^N \backslash E} [\log(\rho_1 + s w_0) - \log M] w_0 dx.$$

We have used $w_0 = 0$ in E and $w_1 = 0$ in $\mathbb{R}^N \backslash E$. We now return to the right hand side of the equation above and rewrite it as

$$-s\Big\{ \int_E [\log(\rho_1 - sw_1) - \log \rho_1] w_1 dx + \int_E [\log \rho_1 - \log M] w_1 dx$$

$$+ \int_{\mathbb{R}^N \backslash E} [\log M - \log(\rho_1 + sw_0)] w_0 dx \Big\} =: -s(T_1 + T_2 + T_3).$$

Obviously, $T_2 > 0$. As for T_1, we have that

$$0 \le [-\log(\rho_1 - sw_1) + \log \rho_1] w_1 \le [\log \rho_1 - \log((1-s)\rho_1)] w_1 \le -\rho_1 \log(1-s) \text{ in } E$$

if $0 < s < 1$. Thus, $T_1 \uparrow 0$ as $s \downarrow 0$.
The study of T_3 is next. We write

$$\log M - \log(\rho_1 + sw_0) = \log \frac{M}{\rho_1 + sw_0} \ge -\log(1+s)$$

since both ρ_1 and w_0 are less than M in $\mathbb{R}^N \backslash E$. Consequently, since $w_0 \le \rho_0 \chi_{\mathbb{R}^N \backslash E}$ in $\mathbb{R}^N$,

$$T_3 \ge -\log(1+s) \int_{\mathbb{R}^N} w_0 dx \ge -\log(1+s).$$

Therefore,

$$-s\Big\{ \frac{1}{2\tau} \iint_{(\mathbb{R}^N \backslash E) \times E} |x-y|^2 d\mu(x,y) + T_1 + T_2 + T_3 \Big\} < 0$$

for sufficiently small $s > 0$. The minimality of $I[\rho_0; \tau](\rho_1)$ (by (2.1)) is contradicted, i.e. $0 \le \rho_1 \le M$ a.e. in $\mathbb{R}^N$.

$\square$

Next we show that $\rho_1 \in H^1(\mathbb{R}^N)$ and $\tau \nabla \rho_1(x) = [\nabla \Phi(x) - x] \rho_1(x)$ for a.e. $x \in \mathbb{R}^N$, where $\Phi : \mathbb{R}^N \to \mathbb{R}$ is the convex potential whose a.e. gradient realizes the optimal transportation of $\rho_1 dx$ onto $\rho_0 dx$ [2]. Then, as a consequence of $\rho_1 \in L^\infty(\mathbb{R}^N)$, we infer $\rho_1 \in W^{1,\infty}_{loc}(\mathbb{R}^N)$.

Proposition 3. *For every $\tau > 0$ and every $\rho_0 \in \mathcal{M} \cap L^\infty(\mathbb{R}^N)$, the minimizer ρ_1 of (1.4) lies in $H^1(\mathbb{R}^N)$ and*

$$\nabla \rho_1(x) = \frac{1}{\tau} [\nabla \Phi(x) - x] \rho_1(x) \text{ for a.e. } x \in \mathbb{R}^N, \tag{2.2}$$

where $\Phi : \mathbb{R}^N \to \mathbb{R}$ is the unique $\rho_1 dx$-a.e. convex function such that $\nabla \Phi_{\#} \rho_1 = \rho_0$. Consequently, $\rho_1 \in \mathcal{M} \cap L^\infty(\mathbb{R}^N) \cap H^1(\mathbb{R}^N) \cap W^{1,\infty}_{loc}(\mathbb{R}^N)$.

Proof: The argument is based on analyzing the Euler equation associated to (1.4). According to [7], let $\mu \in P(\rho_0, \rho_1)$ be optimal in the definition of $d(\rho_0, \rho_1)$. Then [7],

$$\iint_{\mathbb{R}^N \times \mathbb{R}^N} (y-x) \cdot \xi(y) d\mu(x,y) - \tau \int_{\mathbb{R}^N} \rho_1(x) \nabla \cdot \xi(x) dx = 0 \text{ for all } \xi \in C_c^\infty(\mathbb{R}^N; \mathbb{R}^N). \tag{2.3}$$

We have

$$\left| \iint_{\mathbb{R}^N\times\mathbb{R}^N} (y-x)\cdot\xi(y)d\mu(x,y)\right| \le \left(\iint_{\mathbb{R}^N\times\mathbb{R}^N} |x-y|^2 d\mu(x,y)\right)^{1/2} \tag{2.4}$$

$$\times\left(\int_{\mathbb{R}^N} \rho_1(y)|\xi(y)|^2 dy\right)^{1/2} \le \|\rho_1\|_\infty^{1/2} d(\rho_0,\rho_1)\|\xi\|_{L^2(\mathbb{R}^N)}.$$

Note that (2.3) and (2.4) imply that ρ_1 has a distributional gradient $\nabla\rho_1 \in L^2(\mathbb{R}^N;\mathbb{R}^N)$ that satisfies

$$\iint_{\mathbb{R}^N\times\mathbb{R}^N} (y-x)\cdot\xi(y)d\mu(x,y) + \tau\int_{\mathbb{R}^N} \nabla\rho_1\cdot\xi dx = 0, \tag{2.5}$$

for all $\xi \in C_c^\infty(\mathbb{R}^N;\mathbb{R}^N)$. In view of (2.4) and (2.5) we obtain

$$\|\nabla\rho_1\|_{L^2(\mathbb{R}^N)} \le \frac{1}{\tau}\|\rho_1\|_\infty^{1/2} d(\rho_0,\rho_1). \tag{2.6}$$

Furthermore [8],

$$\iint_{\mathbb{R}^N\times\mathbb{R}^N} \varphi(x,y)d\mu(x,y) = \int_{\mathbb{R}^N} \rho_1(y)\varphi(\nabla\Phi(y),y)dy \text{ for all } \varphi\in C_c(\mathbb{R}^N\times\mathbb{R}^N).$$

Applying this to $\varphi(x,y) := x\cdot\xi(y)$ gives, via (2.5),

$$\frac{1}{\tau}\big(\nabla\Phi - \mathrm{Id}_{\mathbb{R}^N}\big)\rho_1 - \nabla\rho_1 = 0 \text{ a.e. in } \mathbb{R}^N. \tag{2.7}$$

Since Φ, as a convex function, is locally Lipschitz, the rest of the conclusion follows.

□

Remark: From (2.7) one can easily see that, in fact, $\nabla\rho_1$ also lies in $L^1(\mathbb{R}^N)$ and

$$\begin{aligned}\|\nabla\rho_1\|_{L^1(\mathbb{R}^N)} &= \frac{1}{\tau}\int_{\mathbb{R}^N} \{|\nabla\Phi(x)-x|[\rho_1(x)]^{1/2}\}[\rho_1(x)]^{1/2}dx\\ &\le \frac{1}{\tau}d(\rho_0,\rho_1)\end{aligned}$$

by Hölder's inequality. This leads us to believe that it may be possible to show that $\rho_1 \in W^{1,1}(\mathbb{R}^N)$ without assuming $\rho_1\in L^\infty(\mathbb{R}^N)$ which comes as a consequence of $\rho_0\in L^\infty(\mathbb{R}^N)$ (Proposition 2).

2.2 The general case

Next we drop the assumption $\rho_0 \in L^\infty(\mathbb{R}^N)$ and we plan to prove a more general proposition. Let us consider the addition of an extra term to (1.1), namely an energy given by a smooth potential $\psi : \mathbb{R}^N \to [0,\infty)$ satisfying

$$|\nabla\psi(x)| \le C[1+\psi(x)],\ x\in\mathbb{R}^N. \tag{2.8}$$

Thus, we obtain

$$I_\psi[\rho_0;\tau](\rho) := \frac{1}{2\tau}d(\rho,\rho_0)^2 + \int_{\mathbb{R}^N}\psi(x)\rho(x)dx + \int_{\mathbb{R}^N}\rho(x)\log\rho(x)dx \tag{2.9}$$

which is the functional used in [7] to iteratively construct approximants to the solution of the Fokker-Planck IVP

$$\frac{\partial\rho}{\partial t} = \nabla\cdot[\rho\nabla\psi] + \Delta\rho,\ \ \rho(\cdot,0) = \rho_0. \tag{2.10}$$

Although most of our work is concerned with the case $\psi \equiv 0$, a notable exception is the last section, where quadratic potentials are utilized.

Proposition 4. *For every $\tau > 0$ and every $\rho_0 \in \mathcal{M}$, the minimizer ρ_1 of (2.9) over $\mathcal{M}$ lies in $W^{1,1}(\mathbb{R}^N)$ and*

$$\nabla\rho_1(x) = \left\{\frac{1}{\tau}[\nabla\Phi(x) - x] - \nabla\psi(x)\right\}\rho_1(x) \text{ for a.e. } x \in \mathbb{R}^N, \tag{2.11}$$

where $\Phi : \mathbb{R}^N \to \mathbb{R}$ is the unique $\rho_1 dx$-a.e. convex function such that $\nabla\Phi_{\#}\rho_1 = \rho_0$. Furthermore, the function $\tilde\rho : \mathbb{R}^N \to (0,\infty)$ given by

$$\tilde\rho(x) := \exp\left\{\frac{1}{\tau}\left[-\frac{|x|^2}{2} + \Phi(x)\right] - \psi(x)\right\}$$

is integrable in $\mathbb{R}^N$ and

$$\rho_1(x) = \tilde\rho(x)\Big/\int_{\mathbb{R}^N}\tilde\rho(y)dy \text{ for a.e. } x \in \mathbb{R}^N. \tag{2.12}$$

Let us begin with a lemma. This may very well be folklore but we were not able to find it anywhere.

Lemma 1. *Let $\Omega \subset \mathbb{R}^N$ be bounded with Lipschitz boundary. If $f \in W^{1,1}(\Omega)$ and $g \in W^{1,\infty}(\Omega)$, then $fg \in W^{1,1}(\Omega)$ and $\nabla(fg) = f\nabla g + g\nabla f$.*

Proof: There exists [5] a sequence $\{f_n\}_n \subset W^{1,1}(\Omega)\cap C^\infty(\overline{\Omega})$ such that $f_n \to f$ in $W^{1,1}(\Omega)$. Since $f_n,\ g \in W^{1,1}(\Omega)\cap L^\infty(\Omega)$, it follows [5] $f_n g \in W^{1,1}(\Omega)\cap L^\infty(\Omega)$ and $\nabla(f_n g) = f_n\nabla g + g\nabla f_n$ which is equivalent to

$$-\int_{\mathbb{R}^N}(f_n g)\nabla\psi dx = \int_{\mathbb{R}^N}(\psi f_n)\nabla g dx + \int_{\mathbb{R}^N}(\psi g)\nabla f_n dx \text{ for all } \psi \in C_c^\infty(\Omega).$$

Since $g\nabla\psi,\ \psi\nabla g$ and ψg are essentially bounded in Ω and $f_n \to f$ in $W^{1,1}(\Omega)$, we may pass to the limit to obtain

$$-\int_{\mathbb{R}^N}(fg)\nabla\psi dx = \int_{\mathbb{R}^N}(\psi f)\nabla g dx + \int_{\mathbb{R}^N}(\psi g)\nabla f dx \text{ for all } \psi \in C_c^\infty(\Omega),$$

i.e. $\nabla(fg) = f\nabla g + g\nabla f$ as distributions. As $f\nabla g,\ g\nabla f \in L^1(\Omega;\mathbb{R}^N)$, the proof is concluded.

□

We are now ready to prove Proposition 4.
Proof of Proposition 4: First of all, note that a more general version (2.3) is valid independently of the assumption $\rho_0 \in L^\infty(\mathbb{R}^N)$. More precisely [7],

$$\iint_{\mathbb{R}^N\times\mathbb{R}^N} (y-x)\cdot\xi(y)d\mu(x,y) - \tau\int_{\mathbb{R}^N} \rho_1(x)[\nabla\cdot\xi(x) - \nabla\psi(x)\cdot\xi(x)]dx = 0 \tag{2.13}$$

for all $\xi \in C_c^\infty(\mathbb{R}^N;\mathbb{R}^N)$. Thus, just as in establishing (2.7), we infer that (2.11) holds for the distributional gradient of ρ_1 (the only difference is that, in general, $\nabla\rho_1$ is not a square-integrable function).
Since ρ_1 is a probability density in $\mathbb{R}^N$, for $R > 0$ large enough we have

$$1 \geq \int_{\mathcal{B}_R} \rho_1 dx =: \alpha_R > 0, \text{ where } \mathcal{B}_R := \big\{x\in\mathbb{R}^N \;\big|\; |x|\leq R\big\}. \tag{2.14}$$

In what follows, $f\lfloor R$ denotes the restriction to $\mathcal{B}_R$ of a function f defined on $\mathbb{R}^N$.
Since Φ is convex and ψ is smooth in $\mathbb{R}^N$ satisfying (2.8),

$$g := \frac{1}{\tau}\left(\Phi\lfloor R - \frac{1}{2}|\mathrm{Id}|^2\lfloor R\right) - \psi\lfloor R \in W^{1,\infty}(\mathcal{B}_R).$$

This implies

$$e^{-g} \in W^{1,\infty}(\mathcal{B}_R) \text{ and } \nabla\rho_1\lfloor R = \frac{1}{\tau}(\rho_1\lfloor R)\nabla g \in L^1(\mathcal{B}_R;\mathbb{R}^N).$$

Thus,

$$e^{-g} \in W^{1,\infty}(\mathcal{B}_R) \text{ and } \rho_1\lfloor R \in W^{1,1}(\mathcal{B}_R).$$

Lemma 1 applies to yield

$$e^{-g}(\rho_1\lfloor R) \in W^{1,1}(\mathcal{B}_R)$$

and

$$\nabla\big[e^{-g}(\rho_1\lfloor R)\big] = e^{-g}\left[\nabla\rho_1\lfloor R - \frac{1}{\tau}(\rho_1\lfloor R)\nabla g\right] = 0 \text{ a.e. in } \mathcal{B}_R.$$

Along with (2.14), the last equation leads to

$$\rho_1\lfloor R = \alpha_R e^g \Big/ \int_{\mathcal{B}_R} e^g dy \text{ a.e. in } \mathcal{B}_R.$$

We now let $R\uparrow\infty$ and note that $\alpha_R\uparrow 1$ to conclude the proof.

$\square$

Remark: Thus, we have $\rho_1 \in \mathcal{M}\cap W^{1,1}(\mathbb{R}^N)\cap W^{1,\infty}_{loc}(\mathbb{R}^N)$ because Φ is locally Lipschitz. Recall that if ρ_0 is essentially bounded, then ρ_1 gains some extra regularity, more precisely $\rho_1 \in \mathcal{M}\cap L^\infty(\mathbb{R}^N)\cap H^1(\mathbb{R}^N)\cap W^{1,1}(\mathbb{R}^N)\cap W^{1,\infty}_{loc}(\mathbb{R}^N)$. However, as we shall see in the next section,

$$\rho_1 \in \mathcal{M}\cap W^{1,1}(\mathbb{R}^N)\cap W^{1,\infty}_{loc}(\mathbb{R}^N) \tag{2.15}$$

is enough for our purposes.

3 The main result

Let us begin with a lemma.

Lemma 2. *Let* $\Psi : \mathbb{R}^N \to \mathbb{R}$ *be convex and* $f \in L^1(\mathbb{R}^N) \cap W^{1,\infty}_{loc}(\mathbb{R}^N)$ *be nonnegative (of positive total mass). Also, suppose* $|\nabla\Psi| f \in L^1(\mathbb{R}^N)$ *and* $\nabla\Psi \cdot \nabla f \in L^1(\mathbb{R}^N)$*. Then,*

$$\int_{\mathbb{R}^N} \nabla\Psi \cdot \nabla f dx \leq 0. \tag{3.1}$$

Proof: Let $0 < R < \infty$. By a standard mollification (mollify f) argument we obtain

$$-\int_{\mathcal{B}_R} \nabla\Psi \cdot \nabla f dx = \int_{\mathcal{B}_R} f d[\Delta\Psi] - \int_{\partial\mathcal{B}_R} f[\nu \cdot \mathcal{T}_R(\nabla\Psi)] d\mathcal{H}^{N-1}, \tag{3.2}$$

where $[\Delta\Psi]$ is a nonnegative Radon measure (due to the convexity of Ψ) and $\mathcal{T}_R$ is the trace operator defined on $BV(\mathcal{B}_R)$ with values in $L^1(\partial\mathcal{B}_R)$, linear and continuous [5]. By dominated convergence,

$$\int_{\mathcal{B}_R} \nabla\Psi \cdot \nabla f dx \to \int_{\mathbb{R}^N} \nabla\Psi \cdot \nabla f dx \text{ as } R \uparrow \infty$$

and

$$\int_{\mathcal{B}_R} f d[\Delta\Psi] \to \int_{\mathbb{R}^N} f d[\Delta\Psi] \text{ as } R \uparrow \infty$$

by monotone convergence.
Suppose (3.1) is false. Then, (3.2) implies there exists

$$\lim_{R\uparrow\infty} \int_{\partial\mathcal{B}_R} f[\nu \cdot \mathcal{T}_R(\nabla\Psi)] d\mathcal{H}^{N-1} =: L \in (0, \infty]. \tag{3.3}$$

Next we claim that

$$\text{for } \mathcal{L}^1\text{-a.e. } R > 0 \text{ we have } \mathcal{T}_R(\nabla\Psi) = \nabla\Psi,\ \mathcal{H}^{N-1}\text{-a.e. on } \partial\mathcal{B}_R. \tag{3.4}$$

Indeed, according to the Lebesgue-Besicovitch differentiation theorem, we have

$$\nabla\Psi(x) = \lim_{r\downarrow 0} Avg \int_{\mathcal{B}(x,r)} \nabla\Psi(y) dy,\ \mathcal{L}^N\text{-a.e. } x \in \mathbb{R}^N$$

since $\nabla\Psi \in L^\infty_{loc}(\mathbb{R}^N;\mathbb{R}^N) \subset L^1_{loc}(\mathbb{R}^N;\mathbb{R}^N)$. On the other hand, $\nabla\Psi \in BV_{loc}(\mathbb{R}^N;\mathbb{R}^N)$ implies [5]

$$\mathcal{T}_R(\nabla\Psi)(x) = \lim_{r\downarrow 0} Avg \int_{\mathcal{B}(x,r)\cap\mathcal{B}_R} \nabla\Psi(y) dy,\ \mathcal{H}^{N-1}\text{-a.e. } x \in \partial\mathcal{B}_R \text{ for all } R > 0.$$

Thus, (3.4) is verified. Combined with (3.3), it delivers

$$\lim_{R\uparrow\infty} \int_{\partial\mathcal{B}_R} f(\nu \cdot \nabla\Psi) d\mathcal{H}^{N-1} =: L \in (0, \infty]$$

which contradicts the hypothesis that $|\nabla\Psi|f \in L^1(\mathbb{R}^N)$, i.e. (as a consequence of the co-area formula)

$$\int_{\mathbb{R}^N} |\nabla\Psi| f dx = \int_0^\infty \Big(\int_{\partial\mathcal{B}_R} |\nabla\Psi| f d\mathcal{H}^{N-1} \Big) dR < +\infty.$$

□

We are now ready to prove Theorem 1.

Proof of Theorem 1: Note that

$$\int_{\mathbb{R}^N} |x|^2 \rho_1(x)dx - \int_{\mathbb{R}^N} |x|^2 \rho_0(x)dx = \int_{\mathbb{R}^N} [|x|^2 - |\nabla\Phi(x)|^2]\rho_1(x)dx$$

due to $\nabla\Phi_{\#}\rho_1 = \rho_0$. Thus,

$$\begin{aligned}\int_{\mathbb{R}^N} |x|^2 \rho_1(x)dx - \int_{\mathbb{R}^N} |x|^2 \rho_0(x)dx &= -\int_{\mathbb{R}^N} [x + \nabla\Phi(x)] \cdot \{[\nabla\Phi(x) - x]\rho_1(x)\}dx \\ &= -\tau \int_{\mathbb{R}^N} [x + \nabla\Phi(x)] \cdot \nabla\rho_1(x)dx. \qquad (3.5)\end{aligned}$$

Since $\rho_0,\ \rho_1 \in \mathcal{M}$ and $\tau\nabla\rho_1 = [\nabla\Phi - \mathrm{Id}]\rho_1$ a.e. in $\mathbb{R}^N$, we deduce $\mathrm{Id}\cdot\nabla\rho_1,\ \nabla\Phi\cdot\nabla\rho_1 \in L^1(\mathbb{R}^N)$. As Φ is convex and $\rho_1 \in L^1(\mathbb{R}^N) \cap W^{1,\infty}_{loc}(\mathbb{R}^N)$ is nonnegative of unit mass, Lemma 2 applies to yield

$$\int_{\mathbb{R}^N} \nabla\Phi \cdot \nabla\rho_1 dx \le 0. \qquad (3.6)$$

By mollifying ρ_1 locally (in $\mathcal{B}_R$), we deduce

$$\int_{\mathcal{B}_R} x \cdot \nabla\rho_1(x)dx = \int_{\partial\mathcal{B}_R} \rho_1(y)[\nu(y)\cdot y] d\mathcal{H}^{N-1}(y) - N \int_{\mathcal{B}_R} \rho_1(x)dx$$

for every $R > 0$. Let $R \uparrow \infty$ and apply dominated convergence to the left hand side and monotone convergence to the last term in the right hand side to infer that the first term in the right hand side has a limit, i.e.

$$\lim_{R\uparrow\infty} R \int_{\partial\mathcal{B}_R} \rho_1(y) d\mathcal{H}^{N-1}(y) = N + \int_{\mathbb{R}^N} x\cdot\nabla\rho_1(x)dx =: l \in \mathbb{R}.$$

The integrability of $|\mathrm{Id}|\rho_1$ implies, again as a consequence of the co-area formula for L^1 functions, that $l = 0$. This, along with (3.5) and (3.6), implies (1.5).

□

We now turn our attention to Proposition 1.

Proof of Proposition 1: It is based on the fact (proved above) that

$$\int_{\mathbb{R}^N} x \cdot \nabla\rho_1(x)dx = -N.$$

Indeed, according to the previous proof,

$$\begin{aligned}\int_{\mathbb{R}^N}|x|^2[\rho_1(x)-\rho_0(x)]dx &= N\tau-\int_{\mathbb{R}^N}\nabla\Phi(x)\cdot[\tau\nabla\rho_1(x)]dx\\ &= N\tau-\int_{\mathbb{R}^N}\nabla\Phi(x)\cdot\{[\nabla\Phi(x)-x]\rho_1(x)\}dx\\ &= N\tau-\int_{\mathbb{R}^N}|x-\nabla\Phi(x)|^2\rho_1(x)dx-\int_{\mathbb{R}^N}x\cdot[\nabla\Phi(x)-x]\rho_1(x)dx\\ &= N\tau-d(\rho_0,\rho_1)^2-\tau\int_{\mathbb{R}^N}x\cdot\nabla\rho_1(x)dx\\ &= 2N\tau-d(\rho_0,\rho_1)^2.\end{aligned}$$

□

4 Further remarks

One obvious consequence of (1.5) is that the strict inequality (1.3) is always true. Still, is it possible to have equality in (1.5) (along with 1.7)) and, if that is the case, when does that happen? Retracing the proof of Theorem 1, we discover that we obtain equality in (1.5) if and only if

$$\int_{\mathbb{R}^N}\nabla\Phi(x)\cdot\nabla\rho_1(x)dx=0. \tag{4.1}$$

According to (3.2) and the subsequent argument, (4.1) implies

$$\lim_{R\uparrow\infty}\int_{\mathcal{B}_R}\rho_1(y)[\nu(y)\cdot\nabla\Phi(y)]d\mathcal{H}^{N-1}(y)=\int_{\mathbb{R}^N}\rho_1(x)d[\Delta\Phi(x)]=L\geq 0. \tag{4.2}$$

The same proof of Lemma 2 applies to yield $L=0$. But $\rho_1>0$ everywhere in $\mathbb{R}^N$ (Proposition 4, (2.12)). Since $[\Delta\Phi]$ is a nonnegative Radon measure, it follows that $[\Delta\Phi]\equiv 0$. Thus, Φ is harmonic in the sense of distributions and the classical regularity theory asserts that Φ is, in fact, smooth and $\Delta\Phi\equiv 0$ in the usual sense. As the only harmonic convex functions are the affine functions, we infer that there exist $a,\ b\in\mathbb{R}^N$ such that

$$\Phi(x)=a\cdot x+b,\ \text{for all } x\in\mathbb{R}^N. \tag{4.3}$$

Note that $\nabla\Phi\equiv a$ forces ρ_0 (independently of what ρ_1 is) to be the Dirac mass accumulated at a, i.e. $\rho_0=\delta_a$. However, there is yet another issue that we need to confront at this point. Is Proposition 4 valid if ρ_0 is not necessarily absolutely continuous with respect to $\mathcal{L}^N$, but simply lies in the set

$$\mathcal{P}_2:=\left\{\mu-\text{Borel probability on }\mathbb{R}^N\ \middle|\ \int_{\mathbb{R}^N}|x|^2d\mu(x)<+\infty\right\}?$$

Even before that, do we have a (unique) minimizer $\rho_1 \in \mathcal{M}$ for every $\tau > 0$ and every $\rho_0 \in \mathcal{P}_2$? The answers to these questions are surprisingly simple. It is enough to read the proof [7] of the existence (and uniqueness) of the minimizer in $\mathcal{M}$ to realize that the assumption $\rho_0 \ll \mathcal{L}^N$ is nowhere used; only $\rho_0 \in \mathcal{P}_2$ is essential. Also, the variations used to find the Euler equation (2.3) are the push-forwards of ρ_1 (already proved to exist in $\mathcal{M}$) by a special family of diffeomorphisms of $\mathbb{R}^N$ [7]. Therefore, we can deliver stronger statements. First, the existence of the minimizer ρ_1 of (1.4) in $\mathcal{M}$:

Proposition 5. *Let $\tau > 0$ and $\rho_0 \in \mathcal{P}_2$ be fixed. Then, there exists a unique minimizer in $\mathcal{M}$ of the functional (1.1).*

Secondly, the more general version version of Proposition 4 (with $\psi \equiv 0$):

Proposition 6. *For every $\tau > 0$ and every $\rho_0 \in \mathcal{P}_2$, the minimizer ρ_1 over $\mathcal{M}$ of (1.4) lies in $W^{1,1}(\mathbb{R}^N)$ and*

$$\nabla\rho_1(x) = \frac{1}{\tau}[\nabla\Phi(x) - x]\rho_1(x) \text{ for a.e. } x \in \mathbb{R}^N,$$

where $\Phi : \mathbb{R}^N \to \mathbb{R}$ is the unique $\rho_1 dx$-a.e. convex function such that $\nabla\Phi_{\#}\rho_1 = \rho_0$. Furthermore, the function $\tilde{\rho} : \mathbb{R}^N \to (0, \infty)$ given by

$$\tilde{\rho}(x) := \exp\left\{\frac{1}{\tau}\left[-\frac{|x|^2}{2} + \Phi(x)\right]\right\}$$

is integrable in $\mathbb{R}^N$ and

$$\rho_1(x) = \tilde{\rho}(x) \Big/ \int_{\mathbb{R}^N} \tilde{\rho}(y)dy \text{ for a.e. } x \in \mathbb{R}^N. \tag{4.4}$$

Next we give the stronger version of the main theorem.

Theorem 2. *For every $\rho_0 \in \mathcal{P}_2$ and every $\tau > 0$, the minimizer*

$$\rho_1 := \arg\min_{\rho\in\mathcal{M}} I[\rho_0; \tau](\rho)$$

satisfies

$$\int_{\mathbb{R}^N} |x|^2\rho_1(x)dx \geq N\tau + \int_{\mathbb{R}^N} |x|^2 d\rho_0(x). \tag{4.5}$$

Then, of course:

Proposition 7. *Within the above notation and hypotheses,*

$$\int_{\mathbb{R}^N} |x|^2\rho_1(x)dx - \int_{\mathbb{R}^N} |x|^2 d\rho_0(x) = 2N\tau - d(\rho_0, \rho_1)^2. \tag{4.6}$$

Finally, let us note that, obviously, the conclusion of Corollary 1 holds even for $\rho_0 \in \mathcal{P}_2$. This extended setting allows us to include the cases in which we obtain equality in (4.5) and, implicitly, in (1.7). Indeed, we have seen that the equality in (4.5) forces $\rho_0 = \delta_a$ for some $a \in \mathbb{R}^N$. We can, in fact, state the following:

Proposition 8. *Equality in (4.5) is obtained if and only if*

$$\rho_0 = \delta_a \textit{ for some } a \in \mathbb{R}^N. \tag{4.7}$$

Proof: At this point we only need to show that for every $a \in \mathbb{R}^N$, the probability $\rho_0 = \delta_a$ (which lies in $\mathcal{P}_2$) produces a minimizer ρ_1 over $\mathcal{M}$ such that

$$\int_{\mathbb{R}^N} |x|^2 \rho_1(x)dx = N\tau + \int_{\mathbb{R}^N} |x|^2 d\rho_0(x) = N\tau + |a|^2. \tag{4.8}$$

According to Proposition 6 and (4.4), we have

$$\rho_1(x) = (2\pi\tau)^{-N/2} e^{-|a|^2/(2\tau)} \exp\left\{\frac{1}{\tau}\left[-\frac{|x|^2}{2} + a\cdot x\right]\right\} \text{ for a.e. } x \in \mathbb{R}^N \tag{4.9}$$

which leads to (4.8) after some computation.

□

Remark: Thus, as a byproduct, we have obtained a proof of the fact that the Gaussian centered at a minimizes the energy

$$E(\rho) := \int_{\mathbb{R}^N} \frac{|x-a|^2}{2}\rho(x)dx + \int_{\mathbb{R}^N} \rho(x)\log\rho(x)dx$$

over $\mathcal{M}$. In particular, if $a = 0$, we infer that the steady state of the Fokker-Planck equation

$$\frac{\partial \rho}{\partial t} = \nabla\cdot(x\rho) + \Delta\rho$$

is the minimizer of its corresponding total energy, i.e. the potential energy minus the Gibbs-Boltzmann entropy.

5 Constrained optimization in $\mathcal{M}$

As announced in the introduction, we can now employ (1.3) to prove the existence of a minimizer for (1.1) over $\mathcal{E}_{\theta,u}$ (defined in (1.2)). In this section, we follow the course of action outlined by Carlen and Gangbo in [3].

Let us begin with a useful lemma.

Lemma 3. *Let $\rho_0 \in \mathcal{M}$ and $\tau > 0$ be given. For every $\lambda \geq 0$, denote by $\rho^{(\lambda)}$ the unique minimizer [7] for*

$$I[\rho_0;\tau;\lambda](\rho) := \frac{1}{2\tau}d(\rho,\rho_0)^2 + \int_{\mathbb{R}^N}\rho(x)\log\rho(x)dx + \lambda\int_{\mathbb{R}^N}|x|^2\rho(x)dx, \tag{5.1}$$

over $\mathcal{M}$. Then,

$$\limsup_{\lambda\uparrow\infty} \frac{I[\rho_0;\tau;\lambda](\rho^{(\lambda)})}{\log\lambda} \leq N/2. \tag{5.2}$$

Proof: We have seen (simply take λ instead of $1/(2\tau)$) that the minimizer of

$$\int_{\mathbb{R}^N} \rho(x) \log \rho(x) dx + \lambda \int_{\mathbb{R}^N} |x|^2 \rho(x) dx$$

is the Gaussian

$$G_\lambda(x) = \left(\frac{\lambda}{\pi}\right)^{N/2} \exp\big(-\lambda |x|^2\big), \; x \in \mathbb{R}^N. \tag{5.3}$$

Since $G_\lambda \in \mathcal{M}$, we infer

$$I[\rho_0; \tau; \lambda](\rho^{(\lambda)}) \leq I[\rho_0; \tau; \lambda](G_\lambda).$$

It is an easy computation to show

$$\begin{aligned} I[\rho_0; \tau; \lambda](G_\lambda) &= \frac{1}{2\tau} d(G_\lambda, \rho_0)^2 + \frac{N}{2} \log(\lambda/\pi) \\ &\leq \frac{1}{\tau} \int_{\mathbb{R}^N} |x|^2 \rho_0(x) dx + \frac{1}{\tau} \int_{\mathbb{R}^N} |x|^2 G_\lambda(x) dx + \frac{N}{2} \log(\lambda/\pi) \\ &= \frac{1}{\tau} \int_{\mathbb{R}^N} |x|^2 \rho_0(x) dx + \frac{N \pi^{N/2}}{2\tau \lambda^{1+N/2}} + \frac{N}{2} \log(\lambda/\pi). \end{aligned}$$

Combined with the inequality in the previous display, this leads to (5.2).

□

Next, we show that

Lemma 4. *Let $\rho_0 \in \mathcal{M}$ and $\tau > 0$ be given. Then, there exists some $\lambda_1 > 0$ such that*

$$\int_{\mathbb{R}^N} |x|^2 \rho^{(\lambda_1)}(x) dx \leq \int_{\mathbb{R}^N} |x|^2 \rho_0(x) dx. \tag{5.4}$$

Proof: Suppose

$$\int_{\mathbb{R}^N} |x|^2 \rho^{(\lambda)}(x) dx > \int_{\mathbb{R}^N} |x|^2 \rho_0(x) dx =: m_0, \text{ for all } \lambda > 0.$$

In view of this, the minimizing property of $\rho^{(\lambda)}$ implies (let $\rho = \chi_0$ in (5.1))

$$\frac{1}{2\tau} d(\rho^{(\lambda)}, \rho_0)^2 + \int_{\mathbb{R}^N} \rho^{(\lambda)}(x) \log \rho^{(\lambda)}(x) dx < \frac{1}{2\tau} d(\chi_0, \rho_0)^2 + \frac{N}{2} \log \frac{N}{3m_0} \tag{5.5}$$

for all $\lambda > 0$, where χ_0 is the normalized indicator function of the cube $[0, q]^N$ with $q := (3m_0/N)^{1/2}$ (note that the second order moment of χ_0 is thus m_0). Thus, the left hand side of (5.5) is bounded from above, uniformly with respect to λ. Due to (5.5) and the super-linearity of $\phi(z) = z \log z$, we infer [7] that there exists $\rho^{(\infty)}$ in $\mathcal{M}$ and a subsequence of $\{\rho^{(\lambda)}\}_{\lambda > 0}$ (not relabelled) for $\lambda \uparrow \infty$ such that

$$\rho^{(\lambda)} \rightharpoonup \rho^{(\infty)} \text{ weakly in } L^1(\mathbb{R}^N) \text{ as } \lambda \uparrow \infty.$$

It follows that

$$\int_{\mathbb{R}^N} |x|^2 \rho^{(\infty)}(x)dx \le \liminf_{\lambda\uparrow\infty} \int_{\mathbb{R}^N} |x|^2 \rho^{(\lambda)}(x)dx. \tag{5.6}$$

We also have, since $\rho_1 \in \mathcal{M}$ minimizes $I[\rho_0;\tau]$, that the left hand side of (5.5) is bounded from below by

$$\frac{1}{2\tau} d(\rho_1,\rho_0)^2 + \int_{\mathbb{R}^N} \rho_1(x)\log\rho_1(x)dx = \inf_{\rho\in\mathcal{M}} I[\rho_0](\rho) \in \mathbb{R} \text{ (see [7])} \ ,$$

uniformly with respect to λ. This, in view of (5.5) and (5.6), implies

$$\frac{I[\rho_0;\tau;\lambda](\rho^{(\lambda)})}{\log\lambda} \text{ grows at least as } \frac{\lambda}{\log\lambda}\int_{\mathbb{R}^N} |x|^2 \rho^{(\infty)}(x)dx \text{ as } \lambda\uparrow\infty.$$

Since the integral is strictly positive, we obtain a contradiction to (5.2).

□

We are now in the position to prove

Lemma 5. *Let $\rho_0 \in \mathcal{M}$ and $\tau > 0$ be given. Then, there exists some $\lambda_0 > 0$ such that*

$$\int_{\mathbb{R}^N} |x|^2 \rho^{(\lambda_0)}(x)dx = \int_{\mathbb{R}^N} |x|^2 \rho_0(x)dx. \tag{5.7}$$

Proof: Let $\varphi : [0,\infty) \to \mathbb{R}$ given by

$$\varphi(\lambda) := \int_{\mathbb{R}^N} |x|^2 \rho^{(\lambda)}(x)dx - \int_{\mathbb{R}^N} |x|^2 \rho_0(x)dx.$$

Obviously, (1.3) implies $\varphi(0) > 0$ (in fact, due to (1.5), one has $\varphi(0) \ge N\tau$). Due to Lemma 4, there exists $\lambda_1 > 0$ such that $\varphi(\lambda_1) \le 0$. Therefore, it suffices to know that φ is continuous to deduce (5.7) for some $\lambda_0 \in (0,\lambda_1]$. The minimizing property of $\rho^{(\lambda)}$ is equivalent to

$$I[\rho_0;\tau;\lambda](\rho^{(\lambda)}) \le I[\rho_0;\tau;\lambda](\rho) \tag{5.8}$$

for all $\rho \in \mathcal{M} \cap (L\log L)(\mathbb{R}^N)$. If we let $\lambda \to \lambda^* > 0$, we deduce, again from the superlinearity of $\phi(z) = z\log z$, that there exists $\rho^* \in \mathcal{M}$ such that

$$\rho^{(\lambda)} \rightharpoonup \rho^* \text{ weakly in } L^1(\mathbb{R}^N) \text{ as } \lambda \to \lambda^*$$

up to a subsequence (not relabelled). We refer to [7] once again to write (lower semicontinuity argument)

$$d(\rho^*,\rho_0)^2 \le \liminf_{\lambda\to\lambda^*} d(\rho^{(\lambda)},\rho_0)^2 \text{ and } \int_{\mathbb{R}^N} \rho^*\log\rho^* dx \le \liminf_{\lambda\to\lambda^*} \int_{\mathbb{R}^N} \rho^{(\lambda)}\log\rho^{(\lambda)}dx.$$

According to (5.8), we infer that ρ^* minimizes $I[\rho_0;\tau;\lambda^*]$ over $\mathcal{M}$. But the minimizer is $\rho^{(\lambda^*)}$ and is unique, so $\rho^* \equiv \rho^{(\lambda^*)}$ and the convergence $\rho^{(\lambda)} \rightharpoonup \rho^{(\lambda^*)}$ is true for the whole range of parameters $\lambda \to \lambda^*$. That proves the desired continuity of φ.

□

The next theorem is the motivation of this section and, as explained in the introduction, of the whole paper.

Theorem 3. *For every $\tau > 0$ and every $\rho_0 \in \mathcal{E}_{\theta,0}$ there exists a unique minimizer of (1.1) over $\mathcal{E}_{\theta,0}$.*

Note that we deliberately chose the mean $u = 0 \in \mathbb{R}^N$. For a general $u \in \mathbb{R}^N$, one has to repeat the arguments above with the potential $\psi_u(x) = \lambda|x-u|^2$ instead of $\psi(x) = \lambda|x|^2$.
Proof of Theorem 3: We write down the minimizing property of $\rho^{(\lambda_0)}$ from (5.7). Thus,

$$\frac{1}{2\tau}d(\rho^{(\lambda_0)},\rho_0)^2 + \int_{\mathbb{R}^N}\rho^{(\lambda_0)}\log\rho^{(\lambda_0)}dx + \lambda_0\int_{\mathbb{R}^N}|x|^2\rho^{(\lambda_0)}dx$$
$$\leq \frac{1}{2\tau}d(\rho,\rho_0)^2 + \int_{\mathbb{R}^N}\rho\log\rho dx + \lambda_0\int_{\mathbb{R}^N}|x|^2\rho dx$$

for all $\rho \in \mathcal{M}$. In particular,

$$\frac{1}{2\tau}d(\rho^{(\lambda_0)},\rho_0)^2 + \int_{\mathbb{R}^N}\rho^{(\lambda_0)}\log\rho^{(\lambda_0)}dx \leq \frac{1}{2\tau}d(\rho,\rho_0)^2 + \int_{\mathbb{R}^N}\rho\log\rho dx$$

for all $\rho \in \mathcal{M}$ such that $\int_{\mathbb{R}^N}|x|^2\rho dx = \theta = \int_{\mathbb{R}^N}|x|^2\rho_0 dx$. The only thing left is to show that $\int_{\mathbb{R}^N}x_i\rho^{(\lambda_0)}(x)dx = 0$ for $i = 1,...,N$. To unburden notation, let $\rho_1 := \rho^{(\lambda_0)}$. According to Proposition 4 with the potential $\psi(x) = \lambda_0|x|^2$, $\rho_1 \in W^{1,\infty}_{loc}(\mathbb{R}^N)$ and we may write

$$\int_{\mathcal{B}_R}\frac{\partial\rho_1}{\partial x_i}(x)dx = \int_{\partial\mathcal{B}_R}\rho_1(y)\nu_i(y)d\mathcal{H}^{N-1}(y).$$

Due to (2.11), $\partial\rho_1/\partial x_i \in L^1(\mathbb{R}^N)$. Also, $\rho_1 \in L^1(\mathbb{R}^N)$. Therefore, we can pass to the limit as $R \uparrow \infty$ to deduce

$$\int_{\mathbb{R}^N}\frac{\partial\rho_1}{\partial x_i}(x)dx = 0,\ \ i = 1,...,N.$$

We now integrate (2.11) componentwise to get

$$(2\lambda_0\tau + 1)\int_{\mathbb{R}^N}x_i\rho_1(x)dx - \int_{\mathbb{R}^N}\frac{\partial\Phi}{\partial x_i}(x)\rho_1(x)dx = 0.$$

The proof is concluded by observing that $\nabla\Phi_{\#}\rho_1 = \rho_0$ gives

$$\int_{\mathbb{R}^N}\frac{\partial\Phi}{\partial x_i}(x)\rho_1(x)dx = \int_{\mathbb{R}^N}x_i\rho_0(x)dx = 0.$$

□

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