On the Jordan-Kinderlehrer-Otto variational scheme and constrained optimization in the Wasserstein metric

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Abstract

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. This issue appears in the study of constrained optimization in the 2-Wasserstein metric performed by Carlen and Gangbo for the kinetic Fokker-Planck equation. As an alternative to their duality method, we provide the details of a direct approach, via Lagrange multipliers. Estimates for the fourth-order moments in the constrained case, which are essential to the subsequent alternate analysis, are also obtained.

Keywords. Heat equation, Fokker-Planck equation, kinetic Fokker-Planck equation, discrete variational scheme, discrete approximations, optimal transfer plan, optimal transfer map, convex potential, Wasserstein distance, constrained optimization.

AMS subject classification. 35A15, 35K15, 35Q99, 46E35, 49J45, 49M25.

1 Introduction

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 [9]. The issue appeared in the study of constrained optimization in the 2-Wasserstein and was left open by Carlen and Gangbo in [4]. As an alternative to their duality method, we provide the details of a direct approach, via Lagrange multipliers. We also obtain estimates for the fourth-order moments in the constrained case, which are essential to the subsequent alternate analysis in [5].

Carlen and Gangbo [4] 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 by the same authors in [5] where a kinetic Fokker-Planck equation, related to the Boltzmann equation by the grazing collisions limit, is investigated by means of steepest descent in the Wasserstein metric. The equation reads

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f = \theta \left[\Delta_v f + \nabla_v \cdot \left(\frac{v-u}{\theta} f \right) \right], \tag{1.1}$$

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where

$$u(x) := \int_{\mathbb{R}^N} vF(x,v)\mathrm{d}v \text{ and } \theta(x) := \frac{1}{N}\int_{\mathbb{R}^N} |v-u(x)|^2 F(x,v)\mathrm{d}v$$

are the bulk velocity and the temperature, respectively. We need also define the useful quantity $F(x,v) := f(x,v)/\int_{\mathbb{R}^N} f(x,v)\mathrm{d}v$, which represents the conditional velocity distribution of f at $x \in \mathcal{T}^N$, the N-dimensional torus. The total energy and the momentum of f are, respectively,

$$E[f] := \frac{1}{2}\iint_{\mathcal{T}^N\times\mathbb{R}^N} |v|^2 f(x,v)\mathrm{d}v\mathrm{d}x,\ U[f] := \iint_{\mathcal{T}^N\times\mathbb{R}^N} vf(x,v)\mathrm{d}v\mathrm{d}x.$$

The evolution (1.1) increases the Boltzmann entropy and conserves mass, energy and momentum. Carlen and Gangbo set up a multiple-step implicit variational scheme in the Wasserstein metric, the so-called "splitting scheme" [5], which is adapted to the typical kinetic dynamics of the Boltzmann equation. For the Boltzmann equation, the two basic mechanisms at work are streaming and collisions. In the case of the kinetic Fokker-Planck equation, the collision mechanism is replaced by steepest descent of the relative entropy. The implicit variational scheme implements these mechanisms alternatively at the discrete level. The conservation of the second-order moment (energy) with respect to the velocity variable is not a feature retained by the discrete scheme and can only be proved to hold in the vanishing time-step limit. Discussed in [5] and resolved in the companion paper [4] is a modification of a specific part of the variational scheme (the one accounting for collisions) which imposes conservation of energy even at the discrete level.

Let μ,ν be two probability measures on $\mathbb{R}^N$ with finite second-order moments.

Definition 1. *The Wasserstein distance is defined as*

$$d(\mu,\nu) := \inf_{p\in P(\mu,\nu)}\left(\iint_{\mathbb{R}^N\times\mathbb{R}^N} |x-y|^2\mathrm{d}p(x,y)\right)^{1/2},$$

where $P(\mu,\nu)$ is the set of all Borel probabilities on $\mathbb{R}^N\times\mathbb{R}^N$ with marginals μ and ν, respectively.

Note: By abuse of notation, we use $d(f,g)$ for any two probability densities $f,\ g$ with finite second-order moments to mean the Wasserstein distance between the corresponding probability measures. Likewise, $d(\mu,f)$ may be used for a probability μ and a probability density f (both having finite second-order moments).

Next, we recall the algorithm in [5]. Fix an initial density $f_0(x,v)$ and a time-step $\tau > 0$. For any integer $k \geq 1$, one performs the following steps:

(1) Streaming: let $\tilde{f}_k(x,v) := f_{k-1}(x-\tau v, v)$;

(2) Define: $\tilde{F}_k(x,v) := \tilde{f}_k(x,v)/\int_{\mathbb{R}^N}\tilde{f}_k(x,v)\mathrm{d}v$, then

$$\tilde{u}_k(x) := \int_{\mathbb{R}^N} v\tilde{F}_k(x,v)\mathrm{d}v \text{ and } \tilde{\theta}_k(x) := \frac{1}{N}\int_{\mathbb{R}^N}|v-\tilde{u}_k(x)|^2\tilde{F}_k(x,v)\mathrm{d}v.$$

(3) Collisions: steepest descent of the relative entropy

$$H(G|M) := \int_{\mathbb{R}^N}\frac{G(v)}{M(v)}\log\frac{G(v)}{M(v)}\mathrm{d}M(v).$$

For any x, minimize the functional

$$F \to d^2(\tilde{F}_k(x,\cdot),F) + 2\tau\tilde{\theta}_k(x)H(F|M_{\tilde{F}_k(x,\cdot)})$$

over all densities on $\mathbb{R}^N$ with finite second-order moments. The Maxwellian M_G is given by

$$M_G(v) := (2\pi\theta)^{-N/2} \exp\{-|v-u|^2/(2\theta)\},$$

where u and θ are the bulk velocity and, respectively, the temperature corresponding to G.
(4) Define $f_k(x,v) = F_k(x,v) \int_{\mathbb{R}^N} \tilde{f}_k(x,v)\mathrm{d}v$, where F_k is the minimizer from the previous step.

The authors propose [5] replacing the relative entropy $H(F|M_{\tilde{F}_k(x,\cdot)})$ by simply the negative Boltzmann entropy $H(F) = \int_{\mathbb{R}^N} F \log F \mathrm{d}v$ at step (3) while imposing conservation of energy at the discrete level. Though more natural (on account of the evolution properties), this approach is difficult due the constraint not being closed in the appropriate topology. Furthermore, the analysis subsequent to this change in the discrete scheme requires [4] estimates on the fourth-order moments of the minimizers which now need to be proved for the *constrained variational problem.* Whereas the desired estimates in the unconstrained case (i.e. pertaining to the scheme given above) are quite straightforward consequences of the displacement convexity of the fourth-order moment functional, things turn out to be more subtle in the constrained case. The issue is left open in [4] and we address it successfully towards the end of this paper. To solve the constrained variational problem, the authors of [4] construct an argument based on the dual variational characterization of the Wasserstein distance in a functional setting. Optimization in this setting is often more convenient due to some helpful compactness properties [7]. Thus, it is known [3], [7] that

$$N - \frac{1}{2}d^2(f_0, f) = \inf\left\{ \int_{\mathbb{R}^N} (uf_0 + vf)\mathrm{d}x \;\middle|\; u(x) + v(y) \geq x \cdot y, \; \mathrm{d}f_0(x)\mathrm{d}f(y) \text{ a.e. } \right\}.$$

The optimal pair (u,v) comes from a dual pair of convex functions whose gradients provide the optimal transportation of f_0 onto f and viceversa. The constrained minimization problem can be recast into a maximization problem in terms of (u,v) and some additional parameters acting as Lagrange multipliers. More precisely, denote by $\eta^*(s)$ the exponential e^{s-1}, which is the Legendre transform of $\eta(s) = s\log s$ for $s \geq 0$ and $\eta(s) = +\infty$ if $s < 0$. Then, it is proved in [4] that the constrained minimization problem discussed above is equivalent to the maximization of

$$J(\alpha, \beta; u, v) := (1 + \beta/2)N - \int_{\mathbb{R}^N} uf_0\mathrm{d}x - \tau \int_{\mathbb{R}^N} \eta^*\left(\frac{\alpha \cdot y + \beta|y|^2/2 + v(y)}{\tau}\right)\mathrm{d}y,$$

where $\alpha \in \mathbb{R}^N$ and $\beta \in \mathbb{R}$ act as Lagrange multipliers for the momentum and energy constraints, respectively.
The first open problem left in [4] is, basically, to find a way to circumvent much of the difficulty incurred by this quite involved maximization problem by building on the unconstrained case analyzed in the seminal paper [9]. The rest of this section provides a more detailed account of what we accomplish in this work.

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

$$I[\rho_0; \tau](\rho) := \frac{1}{2\tau}d^2(\rho_0, \rho) + \int_{\mathbb{R}^N} \rho(x)\log\rho(x)\mathrm{d}x, \tag{1.2}$$

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

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

We also define, more generally,

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

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

$$\mathcal{E}_{\theta,u} := \left\{ \nu \in \mathcal{P}_2 \;\middle|\; \int_{\mathbb{R}^N} x \mathrm{d}\nu(x) = u,\ \int_{\mathbb{R}^N} |x-u|^2 \mathrm{d}\nu(x) = \theta \right\} \tag{1.3}$$

and take $\rho_0 \in \mathcal{E}_{\theta,u} \cap \mathcal{M}$, we wish to prove the existence of a minimizer in $\mathcal{E}_{\theta,u} \cap \mathcal{M}$ for $I[\rho_0;\tau]$ defined in (1.2). Since $\mathcal{E}_{\theta,u} \cap \mathcal{M}$ is not closed in the L^1-weak topology, the constrained minimization problem formulated above requires more work than the unconstrained one. However, as it will be seen in the sequel, one can successfully build an argument based on the results in [9]. To explain, the duality argument used in [4], although natural and enlightening, appears complicated and could readily be replaced, as the authors of [4] observe, by an easier one based on Lagrange multipliers if one knew that the unconstrained minimizer $\rho_1 \in \mathcal{M}$ of $I[\rho_0;\tau]$ satisfied

$$\int_{\mathbb{R}^N} |x|^2 \rho_1(x) \mathrm{d}x > \int_{\mathbb{R}^N} |x|^2 \rho_0(x) \mathrm{d}x, \tag{1.4}$$

i.e. the minimization

$$\inf_{\rho \in \mathcal{M}} I[\rho_0;\tau](\rho) \tag{1.5}$$

increased the second-order moments. The inequality (1.4) is only conjectured in [4].

We shall work within a more general setting and instead of $\rho_0 \in \mathcal{M}$ we shall consider some probability μ which is not necessarily absolutely continuous with respect to $\mathcal{L}^N$, but simply lies in $\mathcal{P}_2$. Our motivation will become clear when we analyze the case of equality in (1.6) below.
It is enough to read the proof [9] of the existence (and uniqueness) of the minimizer in $\mathcal{M}$ to realize that the assumption $\mu \ll \mathcal{L}^N$ is nowhere used; only $\mu \in \mathcal{P}_2$ is essential. Therefore, we can deliver stronger statements. First, the existence of the minimizer ρ_1 of (1.5) in $\mathcal{M}$:

Proposition 1. *Let $\tau > 0$ and $\mu \in \mathcal{P}_2$ be fixed. Then, there exists a unique minimizer of $I[\mu;\tau]$ over $\mathcal{M}$.*

Next we give the main theorem.

Theorem 1. *For every $\mu \in \mathcal{P}_2$ and every $\tau > 0$, the minimizer*

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

satisfies

$$\int_{\mathbb{R}^N} |x|^2 \rho_1(x) \mathrm{d}x \geq N\tau + \int_{\mathbb{R}^N} |x|^2 \mathrm{d}\mu(x). \tag{1.6}$$

To see how the constrained problem can be solved based on this observation, the reader may now skip directly to Section 4. The next statement will also be proved.

Proposition 2. *Within the above notation and hypotheses,*

$$\int_{\mathbb{R}^N} |x|^2 \rho_1(x) \mathrm{d}x - \int_{\mathbb{R}^N} |x|^2 \mathrm{d}\mu(x) = 2N\tau - d^2(\mu,\rho_1). \tag{1.7}$$

We then have:

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

$$d^2(\mu,\rho_1) \leq N\tau. \tag{1.8}$$

Section 2 explores the regularity of the unconstrained minimizer ρ_1. We obtain enough regularity to enable us to prove our main result, Theorem 1. This will be done in Section 3. In Section 4 we use Theorem 1 to obtain existence and uniqueness of the minimizer in the constrained manifold. Finally, in Section 5 we obtain an estimate on the fourth-order moments of the minimizers arising from the constrained variational problem, estimate which was conjectured in [4].

2 Regularity of the minimizer

This section is concerned with the regularity of the minimizer. The results will be needed in the next section.

2.1 The general case

Let us consider the addition of an extra term to (1.2), namely an energy given by a smooth potential $\psi : \mathbb{R}^N \to [0, \infty)$ satisfying

$$|\nabla\psi(x)| \leq C[1 + \psi(x)], \ x \in \mathbb{R}^N. \tag{2.1}$$

Thus, for given $\mu \in \mathcal{P}_2$, we obtain

$$I_\psi[\mu; \tau](\rho) := \frac{1}{2\tau} d^2(\mu, \rho) + \int_{\mathbb{R}^N} \psi(x)\rho(x)\mathrm{d}x + \int_{\mathbb{R}^N} \rho(x) \log \rho(x)\mathrm{d}x \tag{2.2}$$

which, in case μ comes from a density ρ_0, is the functional used in [9] to iteratively construct approximations to the solution of the Fokker-Planck IVP

$$\frac{\partial\rho}{\partial t} = \nabla \cdot [\rho\nabla\psi] + \Delta\rho, \ \rho(\cdot, 0) = \rho_0. \tag{2.3}$$

Although most of our work is concerned with the case $\psi \equiv 0$, a notable exception is Section 4, where quadratic potentials are utilized.

Proposition 3. *For every $\tau > 0$ and every $\mu \in \mathcal{P}_2$, the minimizer ρ_1 of (2.2) over $\mathcal{M}$ lies in $W^{1,1}(\mathbb{R}^N)$ and*

$$\nabla\rho_1(x) = \left\{\frac{1}{\tau}[\nabla\Phi(x) - x] - \nabla\psi(x)\right\}\rho_1(x) \text{ for a.e. } x \in \mathbb{R}^N, \tag{2.4}$$

where $\Phi : \mathbb{R}^N \to \mathbb{R}$ is the unique $\rho_1\mathrm{d}x$-a.e. convex function such that $\nabla\Phi_{\#}\rho_1 = \mu$ [3]. 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

$$\rho_1(x) = \tilde{\rho}(x) \Big/ \int_{\mathbb{R}^N} \tilde{\rho}(y)\mathrm{d}y \text{ for a.e. } x \in \mathbb{R}^N. \tag{2.5}$$

Proof: According to [9],

$$\iint_{\mathbb{R}^N\times\mathbb{R}^N} (y - x) \cdot \xi(y)\mathrm{d}p(x, y) - \tau \int_{\mathbb{R}^N} \rho_1(x)[\nabla \cdot \xi(x) - \nabla\psi(x) \cdot \xi(x)]\mathrm{d}x = 0 \tag{2.6}$$

for all $\xi \in C_c^\infty(\mathbb{R}^N; \mathbb{R}^N)$. Furthermore [11],

$$\iint_{\mathbb{R}^N\times\mathbb{R}^N} \varphi(x, y)\mathrm{d}p(x, y) = \int_{\mathbb{R}^N} \rho_1(y)\varphi(\nabla\Phi(y), y)\mathrm{d}y$$

for all $\varphi \in C(\mathbb{R}^N \times \mathbb{R}^N)$ of at most quadratic growth. Applying this to $\varphi(x, y) := x \cdot \xi(y)$ gives, in view of (2.6),

$$\int_{\mathbb{R}^N} \rho_1(x)\nabla \cdot \xi(x)\mathrm{d}x = -\int_{\mathbb{R}^N} \rho_1(x)\left\{\frac{1}{\tau}\big[\nabla\Phi(x) - x\big] - \nabla\psi(x)\right\} \cdot \xi(x)\mathrm{d}x := -\int_{\mathbb{R}^N} U(x) \cdot \xi(x)\mathrm{d}x \tag{2.7}$$

for all $\xi \in C_c^\infty(\mathbb{R}^N;\mathbb{R}^N)$. It is easy to see, by (2.1) and the minimizing property of ρ_1, that $U \in L^1(\mathbb{R}^N;\mathbb{R}^N)$. Thus, $\rho_1 \in W^{1,1}(\mathbb{R}^N)$ and (2.4) holds. Since ρ_1 is a probability density in $\mathbb{R}^N$, for $R > 0$ large enough we have

$$1 \geq \int_{\mathcal{B}_R} \rho_1 \mathrm{d}x =: \alpha_R > 0, \text{ where } \mathcal{B}_R := \big\{x \in \mathbb{R}^N \bigm| |x| \leq R\big\}. \tag{2.8}$$

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 (2.1),

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

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,

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

which allows to infer

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

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 (2.8), the last equation leads to

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

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

2.2 Discrete comparison principle

In this subsection we discuss the case where μ is absolutely continuous with respect to the Lebesgue measure and comes from a density $\rho_0 \in L^\infty(\mathbb{R}^N)$. Our choice of discussing the essentially bounded case resides in the discrete comparison principle that we state and prove next. Although based on earlier work by different authors [1], [6], [11], [12], [14], 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. Also, higher regularity for the minimizer is obtained.

Proposition 4. *If $\rho_0 \in \mathcal{M} \cap L^\infty(\mathbb{R}^N)$, then the minimizer ρ_1 of (1.5) is also essentially bounded in $\mathbb{R}^N$ and satisfies*

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

Proof: Let $\phi(z) = z\log z$ and let $M \geq \|\rho_0\|_\infty$ be fixed. Take $p \in P(\rho_0,\rho_1)$ to be the optimal transfer plan [7], [15], and let $E := \{\rho_1 > M\}$ be assumed to satisfy $|E| > 0$. Then $p((\mathbb{R}^N\backslash E)\times E) > 0$. Otherwise

$$M|E| < \int_E \rho_1 \mathrm{d}x = p(\mathbb{R}^N \times E) = p(E \times E) \leq p(E \times \mathbb{R}^N) = \int_E \rho_0 \mathrm{d}x \leq M|E|,$$

which is a contradiction. Now define w_0 and w_1 by

$$\int_{\mathbb{R}^N} w_0\xi \mathrm{d}x = \iint_{(\mathbb{R}^N\setminus E)\times E} \xi(x)\mathrm{d}p(x,y) \text{ and } \int_{\mathbb{R}^N} w_1\xi \mathrm{d}x = \iint_{(\mathbb{R}^N\setminus E)\times E} \xi(y)\mathrm{d}p(x,y),$$

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 $\xi \in C(\mathbb{R}^N \times \mathbb{R}^N)$)

$$\iint_{\mathbb{R}^N\times\mathbb{R}^N} \xi(x,y)\mathrm{d}p_s(x,y) = \iint_{\mathbb{R}^N\times\mathbb{R}^N} \xi(x,y)\mathrm{d}p(x,y) + s\iint_{(\mathbb{R}^N\setminus E)\times E} \big(\xi(x,x)-\xi(x,y)\big)\mathrm{d}p(x,y),$$

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

$$\begin{aligned}\frac{1}{2\tau}d^2(\rho_0,\rho_s) + \int_{\mathbb{R}^N}\phi(\rho_s)\mathrm{d}x \qquad\qquad (2.9)\\ \le I[\rho_0;\tau](\rho_1) + \int_{\mathbb{R}^N}[\phi(\rho_s)-\phi(\rho_1)]\mathrm{d}x - \frac{s}{2\tau}\iint_{(\mathbb{R}^N\setminus E)\times E}|x-y|^2\mathrm{d}p(x,y)\end{aligned}$$

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

$$\begin{aligned}\int_{\mathbb{R}^N}[\phi(\rho_s)-\phi(\rho_1)]\mathrm{d}x &\le \int_{\mathbb{R}^N}(\rho_s-\rho_1)\log\rho_s\mathrm{d}x\\ &= -s\int_{\mathbb{R}^N}[\log\rho_s - \log M]w\mathrm{d}x\\ &= -s\int_E[\log(\rho_1 - sw_1)-\log M]w_1\mathrm{d}x + s\int_{\mathbb{R}^N\setminus E}[\log(\rho_1+sw_0)-\log M]w_0\mathrm{d}x.\end{aligned}$$

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

$$\begin{aligned}-s\Big\{\int_E[\log(\rho_1 - sw_1)-\log\rho_1]w_1\mathrm{d}x + \int_E[\log\rho_1 - \log M]w_1\mathrm{d}x\\ + \int_{\mathbb{R}^N\setminus E}[\log M - \log(\rho_1+sw_0)]w_0\mathrm{d}x\Big\} =: -s(T_1+T_2+T_3).\end{aligned}$$

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 $\mathbb{R}^N\setminus E$. Consequently, since $w_0 \le \rho_0\chi_{\mathbb{R}^N\setminus E}$ in $\mathbb{R}^N$,

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

Therefore,

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

for sufficiently small $s > 0$. The minimality of $I[\rho_0; \tau](\rho_1)$ (by (2.9)) is contradicted, i.e. $0 \leq \rho_1 \leq M$ a.e. in $\mathbb{R}^N$. QED.

Now it can be shown [11]:

Proposition 5. *For every $\tau > 0$ and every $\rho_0 \in \mathcal{M} \cap L^\infty(\mathbb{R}^N)$, the minimizer ρ_1 of (1.5) lies in $H^1(\mathbb{R}^N)$ and*

$$\nabla \rho_1(x) = \frac{1}{\tau}[\nabla \Phi(x) - x]\rho_1(x) \text{ for a.e. } x \in \mathbb{R}^N, \tag{2.10}$$

where $\Phi : \mathbb{R}^N \to \mathbb{R}$ is the unique $\rho_1 \mathrm{d}x$-a.e. convex function such that $\nabla \Phi_{\#}\rho_1 = \rho_0$ [3]. Consequently, $\rho_1 \in \mathcal{M} \cap L^\infty(\mathbb{R}^N) \cap H^1(\mathbb{R}^N) \cap W^{1,\infty}_{loc}(\mathbb{R}^N)$.

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. Also, if μ comes from an essentially bounded density ρ_0, 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,

$$\rho_1 \in \mathcal{M} \cap W^{1,1}(\mathbb{R}^N) \cap W^{1,\infty}_{loc}(\mathbb{R}^N) \tag{2.11}$$

is enough for our purposes.

3 Monotonicity of the second-order moments

Let us begin by stating a helpful lemma. The result follows by Lemma 10.4.5 in [2].

Lemma 1. *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,*

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

By a standard mollification (mollify f) argument we obtain

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

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 [8]. An elementary proof (omitted here) of Lemma 1 may be given based on (3.2).

We are now ready to prove Theorem 1.

Proof of Theorem 1: Note that

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

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

$$\begin{aligned}\int_{\mathbb{R}^N} |x|^2 \rho_1(x) \mathrm{d}x - \int_{\mathbb{R}^N} |x|^2 \mathrm{d}\mu(x) &= -\int_{\mathbb{R}^N} [x + \nabla \Phi(x)] \cdot \{[\nabla \Phi(x) - x]\rho_1(x)\} \mathrm{d}x \\ &= -\tau \int_{\mathbb{R}^N} [x + \nabla \Phi(x)] \cdot \nabla \rho_1(x) \mathrm{d}x. \end{aligned} \tag{3.3}$$

Since $\mu \in \mathcal{P}_2$, $\rho_1 \in \mathcal{M}$ 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 1 applies to yield

$$\int_{\mathbb{R}^N} \nabla\Phi\cdot\nabla\rho_1 \mathrm{d}x \leq 0. \tag{3.4}$$

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

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

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.

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

The integrability of $|\mathrm{Id}|\rho_1$ implies, as a consequence of the co-area formula for L^1 functions, that $l = 0$. This, along with (3.3) and (3.4), implies (1.6). QED.

We now turn our attention to Proposition 2.
Proof of Proposition 2: It is based on the fact (proved above) that

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

Indeed, according to a previous argument,

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

which concludes our proof. QED.

The next section contains the motivation for our result.

4 Constrained optimization in $\mathcal{M}$

As announced in the introduction, we can now employ (1.4) to prove the existence of a minimizer for (1.2) over $\mathcal{E}_{\theta,u}\cap\mathcal{M}$ (defined in (1.3)). In this section, we follow the course of action outlined by Carlen and Gangbo in [4].

Let us begin with a useful lemma.

Lemma 2. *Let $\rho_0 \in \mathcal{M}$ and $\tau > 0$ be given. For every $\lambda \geq 0$, denote by $\rho^{(\lambda)}$ the unique minimizer [9] for*

$$I[\mu;\tau;\lambda](\rho) := \frac{1}{2\tau} d^2(\mu,\rho) + \int_{\mathbb{R}^N} \rho(x)\log\rho(x)\mathrm{d}x + \lambda \int_{\mathbb{R}^N} |x|^2 \rho(x)\mathrm{d}x, \tag{4.1}$$

over $\mathcal{M}$. Then,

$$\limsup_{\lambda\uparrow\infty} \frac{I[\mu;\tau;\lambda](\rho^{(\lambda)})}{\log\lambda} \leq N/2. \tag{4.2}$$

Proof: According to the remark immediately following Proposition 6 from the next section (simply take λ instead of $1/(2\tau)$), the minimizer of

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

is the Gaussian

$$G_\lambda(x) = \left(\frac{\lambda}{\pi}\right)^{N/2} \exp\bigl(-\lambda|x|^2\bigr),\ x \in \mathbb{R}^N. \tag{4.3}$$

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

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

It is an easy computation to show

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

Combined with the inequality in the previous display, this leads to (4.2). QED.

Next, we show that

Lemma 3. *Let $\mu \in \mathcal{M}$ and $\tau > 0$ be given. Then, there exists some $\lambda_1 > 0$ such that*

$$\int_{\mathbb{R}^N} |x|^2 \rho^{(\lambda_1)}(x)\mathrm{d}x \leq \int_{\mathbb{R}^N} |x|^2 \mathrm{d}\mu(x). \tag{4.4}$$

Proof: We use the unconstrained minimizer ρ_1 of $I[\mu;\tau]$ to write

$$I[\mu;\tau]\bigl(\rho^{(\lambda)}\bigr) \geq I[\mu;\tau](\rho_1) =: m \text{ for all } \lambda > 0.$$

This inequality leads to,

$$\begin{aligned} \int_{\mathbb{R}^N} |x|^2 \rho^{(\lambda)}(x)\mathrm{d}x &= \frac{1}{\lambda}\Bigl\{ I[\mu;\tau;\lambda] - I[\mu;\tau]\bigl(\rho^{(\lambda)}\bigr)\Bigr\} \\ &\leq \frac{\log\lambda}{\lambda}\frac{I[\mu;\tau;\lambda] - m}{\lambda}. \end{aligned}$$

According to Lemma 2, we deduce

$$\limsup_{\lambda\uparrow\infty} \int_{\mathbb{R}^N} |x|^2 \rho^{(\lambda)}(x)\mathrm{d}x = 0, \tag{4.5}$$

which implies the existence of λ_1 satisfying (4.4). QED.

We are now in the position to prove

Lemma 4. *Let $\mu \in \mathcal{M}$ and $\tau > 0$ be given. Then, there exists some $\lambda_0 > 0$ such that*

$$\int_{\mathbb{R}^N} |x|^2 \rho^{(\lambda_0)}(x)\mathrm{d}x = \int_{\mathbb{R}^N} |x|^2 \mathrm{d}\mu(x). \tag{4.6}$$

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

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

Obviously, (1.4) implies $\varphi(0) > 0$ (in fact, due to (1.6), one has $\varphi(0) \geq N\tau$). Due to Lemma 3, there exists $\lambda_1 > 0$ such that $\varphi(\lambda_1) \leq 0$. Therefore, it suffices to know that φ is continuous to deduce (4.6) for some $\lambda_0 \in (0, \lambda_1]$. The minimizing property of $\rho^{(\lambda)}$ is equivalent to

$$I[\mu;\tau;\lambda](\rho^{(\lambda)}) \leq I[\mu;\tau;\lambda](\rho) \tag{4.7}$$

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 super-linearity 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 [9] once again to write (lower semicontinuity argument)

$$d^2(\mu,\rho^*) \leq \liminf_{\lambda\to\lambda^*} d^2(\mu,\rho^{(\lambda)}) \text{ and } \int_{\mathbb{R}^N} \rho^* \log\rho^* \mathrm{d}x \leq \liminf_{\lambda\to\lambda^*} \int_{\mathbb{R}^N} \rho^{(\lambda)} \log\rho^{(\lambda)}\mathrm{d}x.$$

According to (4.7), we infer that ρ^* minimizes $I[\mu;\tau;\lambda^*]$ 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 $\lambda \to \lambda^*$. Let $f_s := \left[(1-s)\mathrm{id}_{\mathbb{R}^N} + s\nabla\Phi^{(\lambda)}\right]_{\#}\rho^{(\lambda)}$ be the McCann's interpolants with $f_0 = \rho^{(\lambda)}$ and $f_1 = \mu$, where $\nabla\Phi^{(\lambda)}$ is the optimal map pushing $\rho^{(\lambda)}$ forward to μ. It is now a well-known fact [10] that, in particular (obvious in this case),

$$[0,1] \ni s \to M_4(f_s) := \int_{\mathbb{R}^N} |x|^4 f_s(x)\mathrm{d}x = \int_{\mathbb{R}^N} |(1-s)x + s\nabla\Phi^{(\lambda)}(x)|^4 \rho^{(\lambda)}(x)\mathrm{d}x$$

is convex. Thus,

$$\begin{aligned} M_4(\mu) - M_4(\rho^{(\lambda)}) &\geq \frac{\mathrm{d}}{\mathrm{d}s} \int_{\mathbb{R}^N} |x|^4 f_s(x)\mathrm{d}x\bigg|_{s=0} \\ &= \int_{\mathbb{R}^N} \frac{\mathrm{d}}{\mathrm{d}s}|(1-s)x + s\nabla\Phi^{(\lambda)}(x)|^4\bigg|_{s=0} \rho^{(\lambda)}(x)\mathrm{d}x \\ &= 4\int_{\mathbb{R}^N} \left(|x|^2 x\right)\cdot\left\{\left[\nabla\Phi^{(\lambda)}(x) - x\right]\rho^{(\lambda)}(x)\right\}\mathrm{d}x. \end{aligned}$$

We employ (2.4) for $\psi(x) = \lambda|x|^2$ to obtain

$$\begin{aligned} M_4(\rho^{(\lambda)}) - M_4(\mu) &\leq -4\tau\int_{\mathbb{R}^N} \left(|x|^2 x\right)\cdot\left\{\nabla\rho^{(\lambda)}(x) + 2\lambda x\rho^{(\lambda)}(x)\right\}\mathrm{d}x \\ &= -8\lambda\tau M_4(\rho^{(\lambda)}) + 4(N+2)\tau\int_{\mathbb{R}^N} |x|^2\rho^{(\lambda)}(x)\mathrm{d}x. \end{aligned}$$

The second-order moments of $\rho^{(\lambda)}$ are, obviously, bounded from above uniformly as $\lambda \to \lambda^*$. This, in view of the inequality above, implies that the fourth-order moments $M_4(\rho^{(\lambda)})$ are uniformly bounded. Consequently,

$$\int_{|x|\geq R} |x|^2\rho^{(\lambda)}(x)\mathrm{d}x \leq \frac{C}{R^2} \text{ for some } C > 0 \text{ independent of } \lambda. \tag{4.8}$$

For any $R > 0$, one has

$$\left|\int_{\mathbb{R}^N} |x|^2\rho^{(\lambda)}(x)\mathrm{d}x - \int_{\mathbb{R}^N} |x|^2\rho^*(x)\mathrm{d}x\right| \le \left|\int_{|x|\le R} |x|^2\rho^{(\lambda)}(x)\mathrm{d}x - \int_{|x|\le R} |x|^2\rho^*(x)\mathrm{d}x\right| + \int_{|x|\ge R} |x|^2\rho^{(\lambda)}(x)\mathrm{d}x + \int_{|x|\ge R} |x|^2\rho^*(x)\mathrm{d}x.$$

The last integral in the right hand side tends to zero as $R \uparrow \infty$ and this fact, in view of (4.8) and the weak L^1 convergence of $\rho^{(\lambda)}$ to ρ^*, yields the convergence of the second-order moments, i.e. the continuity of φ. QED.

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

Theorem 2. *For every $\tau > 0$ and every $\mu \in \mathcal{E}_{\theta,0}$ there exists a unique minimizer of $I[\mu;\tau]$ over $\mathcal{E}_{\theta,0} \cap \mathcal{M}$.*

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 2: The uniqueness part follows easily from the convexity of the sets $\mathcal{E}_{\theta,0}$ and $\mathcal{M}$ along with the strict convexity of the functional $I[\mu;\tau]$.
We write down the minimizing property of $\rho^{(\lambda_0)}$ from (4.6). Thus,

$$\frac{1}{2\tau}d^2(\mu,\rho^{(\lambda_0)}) + \int_{\mathbb{R}^N} \rho^{(\lambda_0)}\log\rho^{(\lambda_0)}\mathrm{d}x + \lambda_0\int_{\mathbb{R}^N} |x|^2\rho^{(\lambda_0)}\mathrm{d}x \le \frac{1}{2\tau}d^2(\mu,\rho) + \int_{\mathbb{R}^N} \rho\log\rho\mathrm{d}x + \lambda_0\int_{\mathbb{R}^N} |x|^2\rho\mathrm{d}x$$

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

$$\frac{1}{2\tau}d^2(\mu,\rho^{(\lambda_0)}) + \int_{\mathbb{R}^N} \rho^{(\lambda_0)}\log\rho^{(\lambda_0)}\mathrm{d}x \le \frac{1}{2\tau}d^2(\mu,\rho) + \int_{\mathbb{R}^N} \rho\log\rho\mathrm{d}x$$

for all $\rho \in \mathcal{M}$ such that $\int_{\mathbb{R}^N} |x|^2\rho\mathrm{d}x = \theta = \int_{\mathbb{R}^N} |x|^2\mathrm{d}\mu(x)$. The only thing left is to show that $\int_{\mathbb{R}^N} x_i\rho^{(\lambda_0)}(x)\mathrm{d}x = 0$ for $i = 1,...,N$. To unburden notation, let $\rho_1 := \rho^{(\lambda_0)}$. According to Proposition 3 with the potential $\psi(x) = \lambda_0|x|^2$, $\rho_1 \in W^{1,1}(\mathbb{R}^N)$. As a consequence,

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

We now integrate (2.4) componentwise to get

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

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

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

QED.

One obvious consequence of (1.6) is that the strict inequality (1.4) is always true. Still, is it possible to have equality in (1.6) (along with 1.8)) and, if that is the case, when does that happen? Retracing the proof of Theorem 1, we discover that we obtain equality in (1.6) if and only if

$$\int_{\mathbb{R}^N} \nabla\Phi(x) \cdot \nabla\rho_1(x)\mathrm{d}x = 0. \tag{4.9}$$

According to (3.2), (4.9) implies

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

But $L = 0$, because else

$$\liminf_{R\uparrow\infty} \int_{\partial\mathcal{B}_R} \rho_1(y)|\mathcal{T}_R(\nabla\Phi)(y)|\mathrm{d}\mathcal{H}^{N-1}(y) > 0$$

which, by the co-area formula, contradicts $|\nabla\Phi|\rho_1 \in L^1(\mathbb{R}^N)$. Since $\rho_1 > 0$ everywhere in $\mathbb{R}^N$ (Proposition 3, (2.5)) and $[\Delta\Phi]$ 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

$$\Phi(x) = a \cdot x + b, \text{ for all } x \in \mathbb{R}^N. \tag{4.10}$$

Note that $\nabla\Phi \equiv a$ forces μ (independently of what ρ_1 is) to be the Dirac mass accumulated at a, i.e. $\mu = \delta_a$. We can, in fact, state the following:

Proposition 6. *Equality in (1.6) is obtained if and only if*

$$\mu = \delta_a \textit{ for some } a \in \mathbb{R}^N. \tag{4.11}$$

Proof: Necessity was proved when we obtained (4.10). At this point we only need to show that for every $a \in \mathbb{R}^N$, the probability $\mu = \delta_a$ (which lies in $\mathcal{P}_2$) produces a minimizer ρ_1 over $\mathcal{M}$ such that

$$\int_{\mathbb{R}^N} |x|^2\rho_1(x)\mathrm{d}x = N\tau + \int_{\mathbb{R}^N} |x|^2\mathrm{d}\mu(x) = N\tau + |a|^2. \tag{4.12}$$

According to Proposition 3 and (2.5), we have

$$\rho_1(x) = (2\pi\tau)^{-N/2}e^{-|a|^2/(2\tau)}\exp\left\{\frac{1}{\tau}\left[-\frac{|x|^2}{2} + a \cdot x\right]\right\} \text{ for a.e. } x \in \mathbb{R}^N \tag{4.13}$$

which leads to (4.12) after some computation. QED.

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

$$E(\rho) := \frac{1}{2}\int_{\mathbb{R}^N} |x - a|^2\rho(x)\mathrm{d}x + \int_{\mathbb{R}^N} \rho(x)\log\rho(x)\mathrm{d}x$$

over $\mathcal{M}$ (see, e.g., [13]). 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 The fourth-order moments

The other question raised in [4] was whether an inequality of the form

$$\int_{\mathbb{R}^N} |x|^4 \rho_1(x)\mathrm{d}x \le (1 + C\tau) \int_{\mathbb{R}^N} |x|^4 \mathrm{d}\mu(x) \tag{5.1}$$

could be proved for the *constrained minimization problem* (where C may depend on some higher moments of μ). We thank Carlen and Gangbo for clarifying this, since there seems to be an ambiguity at end of the paper [4]. Indeed, the text conveys the impression that the desired estimate should be proved for the *unconstrained minimization problem*, i.e. the JKO variational problem. Note that such estimate is obtained in [5] as an application of McCann's *displacement convexity*. A similar estimate for the constrained case would be necessary if one considered replacing the discrete scheme in [5] by the constrained one, as explained in the introduction.
For now, let us turn our attention to (5.1). The result we prove is stronger than (5.1) and is given next.

Proposition 7. *For every $\mu \in \mathcal{E}_{N\theta,0}$ and every $\tau > 0$, the minimizer*

$$\rho_1 := \arg \min_{\rho \in \mathcal{E}_{N\theta,0} \cap \mathcal{M}} I[\mu; \tau\theta](\rho)$$

satisfies

$$(1 + 2\tau) \int_{\mathbb{R}^N} |x|^4 \rho_1(x)\mathrm{d}x < \int_{\mathbb{R}^N} |x|^4 \mathrm{d}\mu(x) + 4N(N+2)\theta^2\tau. \tag{5.2}$$

Note that $I[\mu; \tau\theta]$ replaces $I[\mu; \tau]$ in the statement above. We do this to be consistent with [4].
A helpful tool is provided by the following lemma.

Lemma 5. *For every $\mu \in \mathcal{E}_{N\theta,0}$ and every $\tau > 0$, the minimizer*

$$\rho_1 := \arg \min_{\rho \in \mathcal{E}_{N\theta,0} \cap \mathcal{M}} I[\mu; \tau\theta](\rho)$$

satisfies

$$d^2(\mu, \rho_1) < N\theta\tau. \tag{5.3}$$

Thus, the equivalent of (1.8) for the constrained problem is also true (with, as noted above, $\tau\theta$ instead of τ).
Proof of Lemma 5: Let Φ be the convex function such that $\nabla\Phi_{\#}\rho_1 = \mu$. According to Theorem 4.1 (with the only exception that, here, μ is only a probability in $\mathcal{P}_2$; however, nothing needs to be changed in the proof in [4] to infer that everything still works in this general case), the Euler equation for the constrained problem leads to, after adapting notation and some manipulation, the following expression for the distributional gradient of ρ_1

$$\nabla\rho_1(x) = \frac{1}{\tau\theta}\left\{\nabla\Phi(x) + \left[\frac{d^2(\mu,\rho_1)}{2N\theta} - \tau - 1\right]x\right\}\rho_1(x), \text{ for a.e. } x \in \mathbb{R}^N. \tag{5.4}$$

Thus, by easily adjusting the proof of Proposition 3, we deduce that $\rho_1 \in W^{1,1}(\mathbb{R}^N) \cap W^{1,\infty}(\mathbb{R}^N)$. Next we rewrite (5.4) as

$$[\nabla\Phi(x) - x]\rho_1(x) = \tau\theta\nabla\rho_1(x) + \left[\tau - \frac{d^2(\mu,\rho_1)}{2N\theta}\right]x\rho_1(x) \tag{5.5}$$

and we use this to compute

$$\begin{aligned}\int_{\mathbb{R}^N} |x|^2\rho_1(x)\mathrm{d}x - \int_{\mathbb{R}^N} |x|^2\mathrm{d}\mu(x) &= -\int_{\mathbb{R}^N}[x + \nabla\Phi(x)] \cdot \{[\nabla\Phi(x) - x]\rho_1(x)\}\mathrm{d}x \\ &= -\int_{\mathbb{R}^N}[x + \nabla\Phi(x)] \cdot \left\{\tau\theta\nabla\rho_1(x) + \left[\tau - \frac{d^2(\mu,\rho_1)}{2N\theta}\right]x\rho_1(x)\right\}\mathrm{d}x.\end{aligned}$$

Taking into account that the second order moments of μ and ρ_1 are both equal to $N\theta$, the display above implies

$$0 = N\theta\tau + \frac{d^2(\mu,\rho_1)}{2} - N\theta\tau - \left[\tau - \frac{d^2(\mu,\rho_1)}{2N\theta}\right]\int_{\mathbb{R}^N} x\cdot\nabla\Phi(x)\mathrm{d}x - \tau\theta\int_{\mathbb{R}^N}\nabla\Phi(x)\cdot\nabla\rho_1(x)\mathrm{d}x.$$

For the same reason

$$\int_{\mathbb{R}^N} x\cdot\nabla\Phi(x)\mathrm{d}x = N\theta - \frac{1}{2}d^2(\mu,\rho_1).$$

Lemma 1 applies again to yield the nonnegativity of $\int_{\mathbb{R}^N}\nabla\Phi(x)\cdot\nabla\rho_1(x)\mathrm{d}x$. We infer

$$d^4(\mu,\rho_1) - 2N\theta(2+\tau)d^2(\mu,\rho_1) + 4N^2\theta^2\tau \geq 0. \tag{5.6}$$

If we combine this and the obvious fact that on $\mathcal{E}_{\theta,0}$ we have

$$d^2(\mu,\rho_1) \leq 2\int_{\mathbb{R}^N}|x|^2\mathrm{d}\mu(x) + 2\int_{\mathbb{R}^N}|x|^2\rho_1(x)\mathrm{d}x = 4N\theta,$$

we deduce that $d^2(\mu,\rho_1)$ must be smaller that the smallest root of the quadratic polynomial in $d^2(\mu,\rho_1)$ from (5.6). Thus

$$d^2(\mu,\rho_1) \leq N\theta\big(2+\tau-\sqrt{4+\tau^2}\big)$$

which concludes the proof. QED.

The proof of Proposition 7 becomes now an easy consequence of the displacement convexity of the fourth-moment functional regarded as a functional on the unconstrained manifold. In fact, one can show that this functional is not displacement convex on the constrained manifold. If it were, an improved estimate would eventually be available.
Proof of Proposition 7: Let $f_s := \big[(1-s)\mathrm{id}_{\mathbb{R}^N} + s\nabla\Phi\big]_{\#}\rho_1$ be the McCann's interpolants with $f_0=\rho_1$ and $f_1=\mu$. Using the displacement convexity of M_4 again, we obtain

$$\begin{aligned} M_4(\mu) - M_4(\rho_1) &\geq \frac{\mathrm{d}}{\mathrm{d}s}\int_{\mathbb{R}^N}|x|^4 f_s(x)\mathrm{d}x\bigg|_{s=0} \\ &= \int_{\mathbb{R}^N}\frac{\mathrm{d}}{\mathrm{d}s}|(1-s)x+s\nabla\Phi(x)|^4\bigg|_{s=0}\rho_1(x)\mathrm{d}x \\ &= 4\int_{\mathbb{R}^N}\big(|x|^2x\big)\cdot\big\{\big[\nabla\Phi(x)-x\big]\rho_1(x)\big\}\mathrm{d}x. \end{aligned}$$

We employ (5.5) once again to obtain

$$\begin{aligned} M_4(\rho_1) - M_4(\mu) &\leq -4\int_{\mathbb{R}^N}\big(|x|^2x\big)\cdot\left\{\tau\theta\nabla\rho_1(x) + \left[\tau - \frac{d^2(\mu,\rho_1)}{2N\theta}\right]x\rho_1(x)\right\}\mathrm{d}x \\ &= -4\left[\tau - \frac{d^2(\mu,\rho_1)}{2N\theta}\right]M_4(\rho_1) - 4\tau\theta\int_{\mathbb{R}^N}\big(|x|^2x\big)\cdot\nabla\rho_1(x)\mathrm{d}x. \end{aligned}$$

Due to the regularity of ρ_1 we can integrate by parts in the last integral, then use Lemma 5 to conclude the proof. QED.

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