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THE VARIATIONAL FORMULATION OF THE FOKKER–PLANCK EQUATION*

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In memory of Richard Duffin

Abstract. The Fokker–Planck equation, or forward Kolmogorov equation, describes the evolution of the probability density for a stochastic process associated with an Ito stochastic differential equation. It pertains to a wide variety of time-dependent systems in which randomness plays a role. In this paper, we are concerned with Fokker–Planck equations for which the drift term is given by the gradient of a potential. For a broad class of potentials, we construct a time discrete, iterative variational scheme whose solutions converge to the solution of the Fokker–Planck equation. The major novelty of this iterative scheme is that the time-step is governed by the Wasserstein metric on probability measures. This formulation enables us to reveal an appealing, and previously unexplored, relationship between the Fokker–Planck equation and the associated free energy functional. Namely, we demonstrate that the dynamics may be regarded as a gradient flux, or a steepest descent, for the free energy with respect to the Wasserstein metric.

Key words. Fokker–Planck equation, steepest descent, free energy, Wasserstein metric

AMS subject classifications. 35A15, 35K15, 35Q99, 60J60

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1. Introduction and overview.

The Fokker–Planck equation plays a central role in statistical physics and in the study of fluctuations in physical and biological systems [7, 22, 23]. It is intimately connected with the theory of stochastic differential equations: a (normalized) solution to a given Fokker–Planck equation represents the probability density for the position (or velocity) of a particle whose motion is described by a corresponding Ito stochastic differential equation (or Langevin equation). We shall restrict our attention in this paper to the case where the drift coefficient is a gradient. The simplest relevant physical setting is that of a particle undergoing diffusion in a potential field [23].

It is known that, under certain conditions on the drift and diffusion coefficients, the stationary solution of a Fokker–Planck equation of the type that we consider here satisfies a variational principle. It minimizes a certain convex free energy functional over an appropriate admissible class of probability densities [12]. This free energy functional satisfies an H-theorem: it decreases in time for any solution of the Fokker–Planck equation [22]. In this work, we shall establish a deeper, and apparently previously unexplored, connection between the free energy functional and the Fokker–Planck dynamics. Specifically, we shall demonstrate that the solution of the

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Fokker–Planck equation follows, at each instant in time, the direction of steepest descent of the associated free energy functional.

The notion of a steepest descent, or a gradient flux, makes sense only in context with an appropriate metric. We shall show that the required metric in the case of the Fokker–Planck equation is the Wasserstein metric (defined in section 3) on probability densities. As far as we know, the Wasserstein metric cannot be written as an induced metric for a metric tensor (the space of probability measures with the Wasserstein metric is not a Riemannian manifold). Thus, in order to give meaning to the assertion that the Fokker–Planck equation may be regarded as a steepest descent, or gradient flux, of the free energy functional with respect to this metric, we switch to a discrete time formulation. We develop a discrete, iterative variational scheme whose solutions converge, in a sense to be made precise below, to the solution of the Fokker–Planck equation. The time-step in this iterative scheme is associated with the Wasserstein metric. For a different view on the use of implicit schemes for measures, see [6, 16].

For the purpose of comparison, let us consider the classical diffusion (or heat) equation

$$\frac{\partial \rho(t,x)}{\partial t} = \Delta \rho(t,x)\,, \quad t \in (0,\infty)\,, \quad x \in \mathbb{R}^n\,,$$

which is the Fokker–Planck equation associated with a standard n-dimensional Brownian motion. It is well known (see, for example, [5, 24]) that this equation is the gradient flux of the Dirichlet integral $\frac{1}{2}\int_{R^n} |\nabla \rho|^2 \, dx$ with respect to the $L^2(\mathbb{R}^n)$ metric. The classical discretization is given by the scheme

$$\left.\begin{array}{l} \text{Determine } \rho^{(k)} \text{ that minimizes} \\[2mm] \frac{1}{2}\,\|\rho^{(k-1)} - \rho\|^2_{L^2(R^n)} \;+\; \frac{h}{2}\displaystyle\int_{R^n} |\nabla \rho|^2 \, dx \end{array}\right\}$$

over an appropriate class of densities ρ. Here, h is the time step size. On the other hand, we derive as a special case of our results below that the scheme

$$\left.\begin{array}{l} \text{Determine } \rho^{(k)} \text{ that minimizes} \\[2mm] \quad \frac{1}{2}\, d(\rho^{(k-1)}, \rho)^2 \;+\; h\displaystyle\int_{\mathbb{R}^n} \rho \log \rho \, dx \\[2mm] \text{over all } \rho \in K\,, \end{array}\right\} \tag{1}$$

where K is the set of all probability densities on $\mathbb{R}^n$ having finite second moments, is also a discretization of the diffusion equation when d is the Wasserstein metric. In particular, this allows us to regard the diffusion equation as a steepest descent of the functional $\int_{\mathbb{R}^n} \rho \log \rho \, dx$ with respect to the Wasserstein metric. This reveals a novel link between the diffusion equation and the Gibbs–Boltzmann entropy $(-\int_{R^n} \rho \log \rho \, dx)$ of the density ρ. Furthermore, this formulation allows us to attach a precise interpretation to the conventional notion that diffusion arises from the tendency of the system to maximize entropy.

The connection between the Wasserstein metric and dynamical problems involving dissipation or diffusion (such as strongly overdamped fluid flow or nonlinear diffusion equations) seems to have first been recognized by Otto in [19]. The results in [19] together with our recent research on variational principles of entropy and free energy type for measures [12, 11, 15] provide the impetus for the present investigation. The work in [12] was motivated by the desire to model and characterize metastability and hysteresis in physical systems. We plan to explore in subsequent research the relevance of the developments in the present paper to the study of such phenomena. Some preliminary results in this direction may be found in [13, 14].

The paper is organized as follows. In section 2, we first introduce the Fokker–Planck equation and briefly discuss its relationship to stochastic differential equations. We then give the precise form of the associated stationary solution and of the free energy functional that this density minimizes. In section 3, the Wasserstein metric is defined, and a brief review of its properties and interpretations is given. The iterative variational scheme is formulated in section 4, and the existence and uniqueness of its solutions are established. The main result of this paper—namely, the convergence of solutions of this scheme (after interpolation) to the solution of the Fokker–Planck equation—is the topic of section 5. There, we state and prove the relevant convergence theorem.

2. The Fokker–Planck equation, stationary solutions, and the free energy functional. We are concerned with Fokker–Planck equations having the form

$$\frac{\partial \rho}{\partial t} = \operatorname{div}\left(\nabla \Psi(x)\rho\right) + \beta^{-1}\Delta\rho\,, \quad \rho(x,0) = \rho^0(x), \tag{2}$$

where the potential $\Psi(x) : \mathbb{R}^n \to [0,\infty)$ is a smooth function, $\beta > 0$ is a given constant, and $\rho^0(x)$ is a probability density on $\mathbb{R}^n$. The solution $\rho(t,x)$ of (2) must, therefore, be a probability density on $\mathbb{R}^n$ for almost every fixed time t. That is, $\rho(t,x) \geq 0$ for almost every $(t,x) \in (0,\infty) \times \mathbb{R}^n$, and $\int_{\mathbb{R}^n} \rho(t,x)\, dx = 1$ for almost every $t \in (0,\infty)$.

It is well known that the Fokker–Planck equation (2) is inherently related to the Ito stochastic differential equation [7, 22, 23]

$$dX(t) = -\nabla\Psi(X(t))dt + \sqrt{2\beta^{-1}}\, dW(t)\,, \qquad X(0) = X^0\,. \tag{3}$$

Here, $W(t)$ is a standard n-dimensional Wiener process, and X^0 is an n-dimensional random vector with probability density ρ^0. Equation (3) is a model for the motion of a particle undergoing diffusion in the potential field Ψ. $X(t) \in \mathbb{R}^n$ then represents the position of the particle, and the positive parameter β is proportional to the inverse temperature. This stochastic differential equation arises, for example, as the Smoluchowski–Kramers approximation to the Langevin equation for the motion of a chemically bound particle [23, 4, 17]. In that case, the function Ψ describes the chemical bonding forces, and the term $\sqrt{2\beta^{-1}}\, dW(t)$ represents white noise forces resulting from molecular collisions [23]. The solution $\rho(t,x)$ of the Fokker–Planck equation (2) furnishes the probability density at time t for finding the particle at position x.

If the potential Ψ satisfies appropriate growth conditions, then there is a unique stationary solution $\rho_s(x)$ of the Fokker–Planck equation, and it takes the form of the Gibbs distribution [7, 22]

$$\rho_s(x) = Z^{-1}\exp(-\beta\Psi(x)), \tag{4}$$

where the partition function Z is given by the expression

$$Z = \int_{\mathbb{R}^n} \exp(-\beta\Psi(x))\, dx.$$

Note that, in order for equation (4) to make sense, Ψ must grow rapidly enough to ensure that Z is finite. The probability measure $\rho_s(x)\,dx$, when it exists, is the unique invariant measure for the Markov process $X(t)$ defined by the stochastic differential equation (3).

It is readily verified (see, for example, [12]) that the Gibbs distribution ρ_s satisfies a variational principle—it minimizes over all probability densities on $\mathbb{R}^n$ the free energy functional

$$F(\rho) = E(\rho) + \beta^{-1} S(\rho), \tag{5}$$

where

$$E(\rho) := \int_{\mathbb{R}^n} \Psi \rho \, dx \tag{6}$$

plays the role of an energy functional, and

$$S(\rho) := \int_{\mathbb{R}^n} \rho \log \rho \, dx \tag{7}$$

is the negative of the Gibbs–Boltzmann entropy functional.

Even when the Gibbs measure is not defined, the free energy (5) of a density $\rho(t,x)$ satisfying the Fokker–Planck equation (2) may be defined, provided that $F(\rho^0)$ is finite. This free energy functional then serves as a Lyapunov function for the Fokker–Planck equation: if $\rho(t,x)$ satisfies (2), then $F(\rho(t,x))$ can only decrease with time [22, 14]. Thus, the free energy functional is an H-function for the dynamics. The developments that follow will enable us to regard the Fokker–Planck dynamics as a gradient flux, or a steepest descent, of the free energy with respect to a particular metric on an appropriate class of probability measures. The requisite metric is the Wasserstein metric on the set of probability measures having finite second moments. We now proceed to define this metric.

3. The Wasserstein metric. The Wasserstein distance of order two, $d(\mu_1, \mu_2)$, between two (Borel) probability measures μ_1 and μ_2 on $\mathbb{R}^n$ is defined by the formula

$$d(\mu_1, \mu_2)^2 = \inf_{p \in \mathcal{P}(\mu_1, \mu_2)} \int_{R^n \times R^n} |x - y|^2 \, p(dxdy), \tag{8}$$

where $\mathcal{P}(\mu_1, \mu_2)$ is the set of all probability measures on $\mathbb{R}^n \times \mathbb{R}^n$ with first marginal μ_1 and second marginal μ_2, and the symbol $|\cdot|$ denotes the usual Euclidean norm on $\mathbb{R}^n$. More precisely, a probability measure p is in $\mathcal{P}(\mu_1, \mu_2)$ if and only if for each Borel subset $A \subset \mathbb{R}^n$ there holds

$$p(A \times \mathbb{R}^n) = \mu_1(A), \;\; p(\mathbb{R}^n \times A) = \mu_2(A).$$

Wasserstein distances of order q with q different from 2 may be analogously defined [10]. Since no confusion should arise in doing so, we shall refer to d in what follows as simply the Wasserstein distance.

It is well known that d defines a metric on the set of probability measures μ on R^n having finite second moments: $\int_{\mathbb{R}^n} |x|^2 \mu(dx) < \infty$ [10, 21]. In particular, d satisfies the triangle inequality on this set. That is, if μ_1, μ_2, and μ_3 are probability measures on $\mathbb{R}^n$ with finite second moments, then

$$d(\mu_1, \mu_3) \leq d(\mu_1, \mu_2) + d(\mu_2, \mu_3) \, . \tag{9}$$

We shall make use of this property at several points later on.

We note that the Wasserstein metric may be equivalently defined by [21]

$$d(\mu_1, \mu_2)^2 = \inf \mathbf{E}|X - Y|^2 , \tag{10}$$

where $\mathbf{E}(U)$ denotes the expectation of the random variable U, and the infimum is taken over all random variables X and Y such that X has distribution μ_1 and Y has distribution μ_2. In other words, the infimum is over all possible couplings of the random variables X and Y. Convergence in the metric d is equivalent to the usual weak convergence plus convergence of second moments. This latter assertion may be demonstrated by appealing to the representation (10) and applying the well-known Skorohod theorem from probability theory (see Theorem 29.6 of [1]). We omit the details.

The variational problem (8) is an example of a Monge–Kantorovich mass transference problem with the particular cost function $c(x, y) = |x-y|^2$ [21]. In that context, an infimizer $p^* \in \mathcal{P}(\mu_1, \mu_2)$ is referred to as an optimal transference plan. When μ_1 and μ_2 have finite second moments, the existence of such a p^* for (8) is readily verified by a simple adaptation of our arguments in section 4. For a probabilistic proof that the infimum in (8) is attained when μ_1 and μ_2 have finite second moments, see [10]. Brenier [2] has established the existence of a *one-to-one* optimal transference plan in the case that the measures μ_1 and μ_2 have bounded support and are absolutely continuous with respect to Lebesgue measure. Caffarelli [3] and Gangbo and McCann [8, 9] have recently extended Brenier's results to more general cost functions c and to cases in which the measures do not have bounded support.

If the measures μ_1 and μ_2 are absolutely continuous with respect to the Lebesgue measure, with densities ρ_1 and ρ_2, respectively, we will write $\mathcal{P}(\rho_1, \rho_2)$ for the set of probability measures having first marginal μ_1 and second marginal μ_2. Correspondingly, we will denote by $d(\rho_1, \rho_2)$ the Wasserstein distance between μ_1 and μ_2. This is the situation that we will be concerned with in what follows.

4. The discrete scheme. We shall now construct a time-discrete scheme that is designed to converge in an appropriate sense (to be made precise in the next section) to a solution of the Fokker–Planck equation. The scheme that we shall describe was motivated by a similar scheme developed by Otto in an investigation of pattern formation in magnetic fluids [19]. We shall make the following assumptions concerning the potential Ψ introduced in section 2:

$$\Psi \in C^\infty(\mathbb{R}^n);$$

$$\Psi(x) \;\geq\; 0 \;\text{ for all } x \in \mathbb{R}^n \,; \tag{11}$$

$$|\nabla \Psi(x)| \;\leq\; C\,(\Psi(x) + 1) \;\text{ for all } x \in \mathbb{R}^n \tag{12}$$

for some constant $C < \infty$. Notice that our assumptions on Ψ allow for cases in which $\int_{R^n} \exp(-\beta\Psi)\;dx$ is not defined, so the stationary density ρ_s given by (4) does not exist. These assumptions allow us to treat a wide class of Fokker–Planck equations. In particular, the classical diffusion equation $\frac{\partial \rho}{\partial t} = \beta^{-1}\Delta\rho$, for which $\Psi \equiv$ const., falls into this category. We also introduce the set K of admissible probability densities:

$$K \;:=\; \left\{ \rho\colon \mathbb{R}^n \to [0,\infty) \text{ measurable} \;\middle|\; \int_{\mathbb{R}^n} \rho(x)\,dx = 1 \;,\, M(\rho) < \infty \right\} ,$$

where

$$M(\rho) = \int_{\mathbb{R}^n} |x|^2 \,\rho(x)\,dx \,.$$

With these conventions in hand, we now formulate the iterative discrete scheme:

$$\left.\begin{array}{l} \text{Determine } \rho^{(k)} \text{ that minimizes} \\ \quad \frac{1}{2}\, d(\rho^{(k-1)},\rho)^2 \;+\; h\, F(\rho) \\ \text{over all } \rho \in K\,. \end{array}\right\} \tag{13}$$

Here we use the notation $\rho^{(0)} = \rho^0$. The scheme (13) is the obvious generalization of the scheme (1) set forth in the Introduction for the diffusion equation. We shall now establish existence and uniqueness of the solution to (13).

PROPOSITION 4.1. *Given $\rho^0 \in K$, there exists a unique solution of the scheme* (13).

Proof. Let us first demonstrate that S is well defined as a functional on K with values in $(-\infty, +\infty]$ and that, in addition, there exist $\alpha < 1$ and $C < \infty$ depending only on n such that

$$S(\rho) \;\geq\; -C\;(M(\rho)+1)^{\alpha} \quad \text{for all } \rho \in K\,. \tag{14}$$

Actually, we shall show that (14) is valid for any $\alpha \in (\frac{n}{n+2}, 1)$. For future reference, we prove a somewhat finer estimate. Namely, we demonstrate that there exists a $C < \infty$, depending only on n and α, such that for all $R \geq 0$, and for each $\rho \in K$, there holds

$$\int_{R^n - B_R} |\min\{\rho\,\log\rho, 0\}|\, dx \;\leq\; C\,\left(\frac{1}{R^2+1}\right)^{\frac{(2+n)\,\alpha - n}{2}} \;(M(\rho)+1)^{\alpha}\,, \tag{15}$$

where B_R denotes the ball of radius R centered at the origin in $\mathbb{R}^n$. Indeed, for $\alpha < 1$ there holds

$$|\min\{z\,\log z, 0\}| \;\leq\; C\, z^{\alpha} \quad \text{for all } z \geq 0.$$

Hence by Hölder's inequality, we obtain

$$\begin{aligned} &\int_{R^n - B_R} |\min\{\rho\,\log\rho, 0\}|\, dx \\ &\leq C \int_{R^n - B_R} \rho^{\alpha}\, dx \\ &\leq C \left(\int_{R^n - B_R} \left(\frac{1}{|x|^2+1}\right)^{\frac{\alpha}{1-\alpha}} dx \right)^{1-\alpha} (M(\rho)+1)^{\alpha}\,. \end{aligned}$$

On the other hand, for $\frac{\alpha}{1-\alpha} > \frac{n}{2}$, we have

$$\int_{R^n - B_R} \left(\frac{1}{|x|^2+1}\right)^{\frac{\alpha}{1-\alpha}} dx \;\leq\; C\,\left(\frac{1}{R^2+1}\right)^{\frac{\alpha}{1-\alpha} - \frac{n}{2}}\,.$$

Let us now prove that for given $\rho^{(k-1)} \in K$, there exists a minimizer $\rho \in K$ of the functional

$$K \ni \rho \;\mapsto\; \tfrac{1}{2}\, d(\rho^{(k-1)},\rho)^2 \;+\; h\, F(\rho)\,. \tag{16}$$

Observe that S is not bounded below on K and hence F is not bounded below on K either. Nevertheless, using the inequality

$$M(\rho_1) \;\le\; 2\,M(\rho_0) + 2\,d(\rho_0,\rho_1)^2 \quad \text{for all } \rho_0,\rho_1 \in K \tag{17}$$

(which immediately follows from the inequality $|y|^2 \le 2|x|^2 + 2|x-y|^2$ and from the definition of d) together with (14) we obtain

$$\begin{aligned} &\tfrac{1}{2}\, d(\rho^{(k-1)},\rho)^2 \;+\; h\,F(\rho) \\ &\overset{(17)}{\ge}\; \tfrac{1}{4}\, M(\rho) \;-\; \tfrac{1}{2}\, M(\rho^{(k-1)}) \;+\; h\,S(\rho) \\ &\overset{(14)}{\ge}\; \tfrac{1}{4}\, M(\rho) \;-\; C\,\left(M(\rho)+1\right)^{\alpha} \;-\; \tfrac{1}{2}\, M(\rho^{(k-1)}) \quad \text{for all } \rho \in K\,, \end{aligned} \tag{18}$$

which ensures that (16) is bounded below. Now, let $\{\rho_\nu\}$ be a minimizing sequence for (16). Obviously, we have that

$$\{S(\rho_\nu)\}_\nu \quad \text{is bounded above}\,, \tag{19}$$

and according to (18),

$$\{M(\rho_\nu)\}_\nu \quad \text{is bounded}\,. \tag{20}$$

The latter result, together with (15), implies that

$$\left\{\int_{\mathbb{R}^n} |\min\{\rho_\nu\,\log\rho_\nu, 0\}|\;dx\right\}_\nu \quad \text{is bounded}\,,$$

which combined with (19) yields that

$$\left\{\int_{\mathbb{R}^n} \max\{\rho_\nu\,\log\rho_\nu, 0\}\;dx\right\}_\nu \quad \text{is bounded}\,.$$

As $z \mapsto \max\{z\log z, 0\}$, $z \in [0,\infty)$, has superlinear growth, this result, in conjunction with (20), guarantees the existence of a $\rho^{(k)} \in K$ such that (at least for a subsequence)

$$\rho_\nu \overset{w}{\rightharpoonup} \rho^{(k)} \quad \text{in } L^1(\mathbb{R}^n)\,. \tag{21}$$

Let us now show that

$$S(\rho^{(k)}) \;\le\; \liminf_{\nu\uparrow\infty} S(\rho_\nu)\,. \tag{22}$$

As $[0,\infty) \ni z \mapsto z\log z$ is convex and $[0,\infty) \ni z \mapsto \max\{z\log z, 0\}$ is convex and nonnegative, (21) implies that for any $R < \infty$,

$$\int_{B_R} \rho^{(k)}\,\log\rho^{(k)}\;dx \;\le\; \liminf_{\nu\uparrow\infty} \int_{B_R} \rho_\nu\,\log\rho_\nu\;dx\,, \tag{23}$$

$$\int_{\mathbb{R}^n - B_R} \max\{\rho^{(k)}\log\rho^{(k)}, 0\}\,dx \;\le\; \liminf_{\nu\uparrow\infty} \int_{\mathbb{R}^n - B_R} \max\{\rho_\nu\log\rho_\nu, 0\}\,dx. \tag{24}$$

On the other hand we have according to (15) and (20)

$$\lim_{R\uparrow\infty}\,\sup_{\nu\in\mathbb{N}} \int_{\mathbb{R}^n - B_R} |\min\{\rho_\nu\,\log\rho_\nu, 0\}|\;dx \;=\; 0\,. \tag{25}$$

Now observe that for any $R<\infty$, there holds

$$S(\rho^{(k)}) \;\le\; \int_{B_R} \rho^{(k)} \,\log \rho^{(k)}\; dx \;+\; \int_{R^n - B_R} \max\{\rho^{(k)} \,\log \rho^{(k)}, 0\}\; dx\,,$$

which together with (23), (24), and (25) yields (22).

It remains for us to show that

$$E(\rho^{(k)}) \le \liminf_{\nu\uparrow\infty} E(\rho_\nu)\,, \tag{26}$$

$$d(\rho^{(k-1)},\rho^{(k)})^2 \le \liminf_{\nu\uparrow\infty} d(\rho^{(k-1)},\rho_\nu)^2\,. \tag{27}$$

Equation (26) follows immediately from (21) and Fatou's lemma. As for (27), we choose $p_\nu\in\mathcal{P}(\rho^{(k-1)},\rho_\nu)$ satisfying

$$\int_{R^n\times R^n} |x-y|^2\, p_\nu(dx\,dy) \;\le\; d(\rho^{(k-1)},\rho_\nu)^2 \;+\; \tfrac{1}{\nu}.$$

By (20) the sequence of probability measures $\{\rho_\nu\, dx\}_{\nu\uparrow\infty}$ is tight, or relatively compact with respect to the usual weak convergence in the space of probability measures on $\mathbb{R}^n$ (i.e., convergence tested against bounded continuous functions) [1]. This, together with the fact that the density $\rho^{(k-1)}$ has finite second moment, guarantees that the sequence $\{p_\nu\}_{\nu\uparrow\infty}$ of probability measures on $\mathbb{R}^n\times\mathbb{R}^n$ is tight. Hence, there is a subsequence of $\{p_\nu\}_{\nu\uparrow\infty}$ that converges weakly to some probability measure p. From (21) we deduce that $p\in\mathcal{P}(\rho^{(k-1)},\rho^{(k)})$. We now could invoke the Skorohod theorem [1] and Fatou's lemma to infer (27) from this weak convergence, but we prefer here to give a more analytic proof. For $R<\infty$ let us select a continuous function $\eta_R\colon\mathbb{R}^n\to[0,1]$ such that

$$\eta_R \;=\; 1 \;\text{ inside of } B_R \quad\text{and}\quad \eta_R \;=\; 0 \;\text{ outside of } B_{2R}\,.$$

We then have

$$\left.\begin{aligned}
&\int_{R^n\times R^n} \eta_R(x)\,\eta_R(y)\,|x-y|^2\, p(dx\,dy)\\
&\qquad = \lim_{\nu\uparrow\infty}\int_{R^n\times R^n} \eta_R(x)\,\eta_R(y)\,|x-y|^2\, p_\nu(dx\,dy)\\
&\qquad \le \liminf_{\nu\uparrow\infty} d(\rho^{(k-1)},\rho_\nu)^2
\end{aligned}\right\} \tag{28}$$

for each fixed $R<\infty$. On the other hand, using the monotone convergence theorem, we deduce that

$$\begin{aligned}
d(\rho^{(k-1)},\rho^{(k)})^2 &\le \int_{R^n\times R^n} |x-y|^2\, p(dx\,dy)\\
&= \lim_{R\uparrow\infty}\int_{R^n\times R^n} \eta_R(x)\,\eta_R(y)\,|x-y|^2\, p(dx\,dy)\,,
\end{aligned}$$

which combined with (28) yields (27).

To conclude the proof of the proposition we establish that the functional (16) has at most one minimizer. This follows from the convexity of K and the strict convexity of (16). The strict convexity of (16) follows from the strict convexity of S, the linearity of E, and the (obvious) convexity over K of the functional $\rho\mapsto d(\rho^{(k-1)},\rho)^2$. $\square$

Remark. One of the referees has communicated to us the following simple estimate that could be used in place of (14)–(15) in the previous and subsequent analysis: for any $\Omega \subset \mathbb{R}^n$ (in particular, for $\Omega = \mathbb{R}^n - B_R$) and for all $\rho \in K$ there holds

$$\int_\Omega |\min\{\rho\log\rho, 0\}|\,dx \le C\int_\Omega \mathrm{e}^{-\frac{|x|}{2}}\,dx + \epsilon M(\rho) + \frac{1}{4\epsilon}\int_\Omega \rho\,dx \tag{29}$$

for any $\epsilon > 0$. To obtain the inequality (29), select $C > 0$ such that for all $z \in [0,1]$, we have $z|\log z| \le C\sqrt{z}$. Then, defining the sets $\Omega_0 = \Omega \cap \{\rho \le \exp(-|x|)\}$ and $\Omega_1 = \Omega \cap \{\exp(-|x|) < \rho \le 1\}$, we have

$$\begin{aligned}\int_\Omega |\min\{\rho\log\rho, 0\}|\,dx &= \int_{\Omega_0} \rho|(\log\rho)_-|\,dx + \int_{\Omega_1} \rho|(\log\rho)_-|\,dx\\ &\le C\int_\Omega \mathrm{e}^{-\frac{|x|}{2}}\,dx + \int_\Omega |x|\rho\,dx\,.\end{aligned}$$

The desired result (29) then follows from the inequality $|x| \le \epsilon|x|^2 + 1/(4\epsilon)$ for $\epsilon > 0$.

5. Convergence to the solution of the Fokker–Planck equation. We come now to our main result. We shall demonstrate that an appropriate interpolation of the solution to the scheme (13) converges to the unique solution of the Fokker–Planck equation. Specifically, the convergence result that we will prove here is as follows.

THEOREM 5.1. *Let $\rho^0 \in K$ satisfy $F(\rho^0) < \infty$, and for given $h > 0$, let $\{\rho_h^{(k)}\}_{k\in\mathbb{N}}$ be the solution of* (13)*. Define the interpolation $\rho_h\colon (0,\infty)\times\mathbb{R}^n \to [0,\infty)$ by*

$$\rho_h(t) \;=\; \rho_h^{(k)} \quad \textit{for } t \in [k\,h, (k+1)\,h) \textit{ and } k \in \mathbb{N}\cup\{0\}.$$

Then as $h \downarrow 0$,

$$\rho_h(t) \;\rightharpoonup\; \rho(t) \quad \textit{weakly in } L^1(\mathbb{R}^n) \quad \textit{for all } t \in (0,\infty)\,, \tag{30}$$

where $\rho \in C^\infty((0,\infty)\times\mathbb{R}^n)$ is the unique solution of

$$\frac{\partial\rho}{\partial t} \;=\; \mathrm{div}(\rho\nabla\Psi) \;+\; \beta^{-1}\Delta\rho\,, \tag{31}$$

with initial condition

$$\rho(t) \;\to\; \rho^0 \quad \textit{strongly in } L^1(\mathbb{R}^n) \quad \textit{for } t \downarrow 0 \tag{32}$$

and

$$M(\rho),\, E(\rho) \;\in\; L^\infty((0,T)) \quad \textit{for all } T < \infty\,. \tag{33}$$

Remark. A finer analysis reveals that

$$\rho_h \;\to\; \rho \quad \textit{strongly in } L^1((0,T)\times\mathbb{R}^n) \quad \textit{for all } T < \infty\,.$$

Proof. The proof basically follows along the lines of [19, Proposition 2, Theorem 3]. The crucial step is to recognize that the first variation of (16) with respect to the independent variables indeed yields a time-discrete scheme for (31), as will now be demonstrated. For notational convenience only, we shall set $\beta \equiv 1$ from here on in. As will be evident from the ensuing arguments, our proof works for any positive β. In fact, it is not difficult to see that, with appropriate modifications to the scheme (13), we can establish an analogous convergence result for time-dependent β.

Let a smooth vector field with bounded support, $\xi \in C_0^\infty(\mathbb{R}^n, \mathbb{R}^n)$, be given, and define the corresponding *flux* $\{\Phi_\tau\}_{\tau \in R}$ by

$$\partial_\tau \Phi_\tau \;=\; \xi \circ \Phi_\tau \quad \text{for all } \tau \in \mathbb{R} \quad \text{and} \quad \Phi_0 \;=\; \mathrm{id}\,.$$

For any $\tau \in \mathbb{R}$, let the measure $\rho_\tau(y)\,dy$ be the *push forward* of $\rho^{(k)}(y)\,dy$ under Φ_τ. This means that

$$\int_{R^n} \rho_\tau(y)\,\zeta(y)\,dy \;=\; \int_{R^n} \rho^{(k)}(y)\,\zeta(\Phi_\tau(y))\,dy \quad \text{for all } \zeta \in C_0^0(\mathbb{R}^n)\,. \tag{34}$$

As Φ_τ is invertible, (34) is equivalent to the following relation for the densities:

$$\det \nabla\Phi_\tau\, \rho_\tau \circ \Phi_\tau \;=\; \rho^{(k)}\,. \tag{35}$$

By (16), we have for each $\tau > 0$

$$\tfrac{1}{\tau}\,\left(\left(\tfrac{1}{2}\,d(\rho^{(k-1)}, \rho_\tau)^2 + h\,F(\rho_\tau)\right) - \left(\tfrac{1}{2}\,d(\rho^{(k-1)}, \rho^{(k)})^2 + h\,F(\rho^{(k)})\right)\right) \;\geq\; 0, \tag{36}$$

which we now investigate in the limit $\tau \downarrow 0$. Because Ψ is nonnegative, equation (34) also holds for $\zeta = \Psi$, i.e.,

$$\int_{R^n} \rho_\tau(y)\,\Psi(y)\,dy \;=\; \int_{R^n} \rho^{(k)}(y)\,\Psi(\Phi_\tau(y))\,dy\,.$$

This yields

$$\tfrac{1}{\tau}\,\left(E(\rho_\tau) - E(\rho^{(k)})\right) \;=\; \int_{R^n} \tfrac{1}{\tau}\,\left(\Psi(\Phi_\tau(y)) - \Psi(y)\right)\,\rho^{(k)}(y)\,dy\,.$$

Observe that the difference quotient under the integral converges uniformly to $\nabla\Psi(y)\cdot\xi(y)$, hence implying that

$$\tfrac{\mathrm{d}}{\mathrm{d}\,\tau}\,\left[E(\rho_\tau)\right]_{\tau=0} \;=\; \int_{R^n} \nabla\Psi(y)\cdot\xi(y)\,\rho^{(k)}(y)\,dy\,. \tag{37}$$

Next, we calculate $\tfrac{\mathrm{d}}{\mathrm{d}\,\tau}\,\left[S(\rho_\tau)\right]_{\tau=0}$. Invoking an appropriate approximation argument (for instance approximating log by some function that is bounded below), we obtain

$$\begin{aligned}
&\int_{R^n} \rho_\tau(y)\,\log(\rho_\tau(y))\,dy \\
&\overset{(34)}{=} \int_{R^n} \rho^{(k)}(y)\,\log(\rho_\tau(\Phi_\tau(y)))\,dy \\
&\overset{(35)}{=} \int_{R^n} \rho^{(k)}(y)\,\log\left(\frac{\rho^{(k)}(y)}{\det\nabla\Phi_\tau(y)}\right)\,dy\,.
\end{aligned}$$

Therefore, we have

$$\tfrac{1}{\tau}\,\left(S(\rho_\tau) - S(\rho^{(k)})\right) \;=\; -\int_{R^n} \rho^{(k)}(y)\,\tfrac{1}{\tau}\,\log(\det \nabla\Phi_\tau(y))\,dy\,.$$

Now using

$$\frac{\mathrm{d}}{\mathrm{d}\tau}[\det\nabla\Phi_\tau(y)]_{\tau=0} \;=\; \mathrm{div}\xi(y)\,,$$

together with the fact that $\Phi_0 = \mathrm{id}$, we see that the difference quotient under the integral converges uniformly to $\mathrm{div}\xi$, hence implying that

$$\frac{\mathrm{d}}{\mathrm{d}\,\tau}\;[S(\rho_\tau)]_{\tau=0} \;=\; -\int_{\mathbb{R}^n} \rho^{(k)}\,\mathrm{div}\xi\;dy\,. \tag{38}$$

Now, let p be optimal in the definition of $d(\rho^{(k-1)},\rho^{(k)})^2$ (see section 3). The formula

$$\int_{R^n\times R^n} \zeta(x,y)\,p_\tau(dx\,dy) = \int_{R^n\times R^n} \zeta(x,\Phi_\tau(y))\,p(dx\,dy)\;,\zeta\in C_0^0(\mathbb{R}^n\times\mathbb{R}^n)$$

then defines a $p_\tau \in \mathcal{P}(\rho^{(k-1)},\rho_\tau)$. Consequently, there holds

$$\begin{aligned}&\tfrac{1}{\tau}\;\left(\tfrac12\,d(\rho^{(k-1)},\rho_\tau)^2 \;-\; \tfrac12\,d(\rho^{(k-1)},\rho^{(k)})^2\right)\\ &\le\; \int_{R^n\times R^n} \tfrac{1}{\tau}\;\left(\tfrac12\,|\Phi_\tau(y)-x|^2 \;-\tfrac12\,|y-x|^2\right)\;p(dx\,dy)\,,\end{aligned}$$

which implies that

$$\begin{aligned}&\limsup_{\tau\downarrow 0}\tfrac{1}{\tau}\;\left(\tfrac12\,d(\rho^{(k-1)},\rho_\tau)^2 \;-\; \tfrac12\,d(\rho^{(k-1)},\rho^{(k)})^2\right)\\ &\le\; \int_{R^n\times R^n}(y-x)\cdot\xi(y)\,p(dx\,dy)\,.\end{aligned} \tag{39}$$

We now infer from (36), (37), (38), and (39) (and the symmetry in $\xi\to-\xi$) that

$$\left.\begin{aligned}&\int_{R^n\times R^n}(y-x)\cdot\xi(y)\,p(dx\,dy) \;+\; h\int_{R^n}\left(\nabla\Psi\cdot\xi-\mathrm{div}\xi\right)\,\rho^{(k)}\;dy \;=\; 0\\ &\text{for all } \xi\in C_0^\infty(\mathbb{R}^n,\mathbb{R}^n)\,.\end{aligned}\right\} \tag{40}$$

Observe that because $p\in\mathcal{P}(\rho^{(k-1)},\rho^{(k)})$, there holds

$$\begin{aligned}&\left|\int_{R^n}(\rho^{(k)}-\rho^{(k-1)})\,\zeta\;dy \;-\; \int_{R^n\times R^n}(y-x)\cdot\nabla\zeta(y)\,p(dx\,dy)\right|\\ &=\;\left|\int_{R^n\times R^n}\left(\zeta(y)-\zeta(x)\;+\;(x-y)\cdot\nabla\zeta(y)\right)p(dx\,dy)\right|\\ &\le\;\tfrac12\,\sup_{R^n}|\nabla^2\zeta|\int_{R^n\times R^n}|y-x|^2\,p(dx\,dy)\\ &=\;\tfrac12\,\sup_{R^n}|\nabla^2\zeta|\,d(\rho^{(k-1)},\rho^{(k)})^2\end{aligned}$$

for all $\zeta\in C_0^\infty(\mathbb{R}^n)$. Choosing $\xi=\nabla\zeta$ in (40) then gives

$$\begin{aligned}&\left|\int_{R^n}\left\{\tfrac{1}{h}\,(\rho^{(k)}-\rho^{(k-1)})\,\zeta+(\nabla\Psi\cdot\nabla\zeta-\Delta\zeta)\;\rho^{(k)}\right\}\;dy\right|\\ &\quad\le\tfrac12\sup_{R^n}|\nabla^2\zeta|\;\tfrac{1}{h}\,d(\rho^{(k-1)},\rho^{(k)})^2\;\;\text{for all}\;\;\zeta\in C_0^\infty(\mathbb{R}^n)\,.\end{aligned} \tag{41}$$

We wish now to pass to the limit $h \downarrow 0$. In order to do so we will first establish the following a priori estimates: for any $T < \infty$, there exists a constant $C < \infty$ such that for all $N \in \mathbb{N}$ and all $h \in [0,1]$ with $N\,h \le T$, there holds

$$M(\rho_h^{(N)}) \le C\,, \tag{42}$$

$$\int_{R^n} \max\{\rho_h^{(N)}\, \log \rho_h^{(N)}, 0\}\, dx \le C\,, \tag{43}$$

$$E(\rho_h^{(N)}) \le C\,, \tag{44}$$

$$\sum_{k=1}^{N} d(\rho_h^{(k-1)}, \rho_h^{(k)})^2 \le C\,h\,. \tag{45}$$

Let us verify that the estimate (42) holds. Since $\rho_h^{(k-1)}$ is admissible in the variational principle (13), we have that

$$\tfrac{1}{2}\, d(\rho_h^{(k-1)}, \rho_h^{(k)})^2 \;+\; h\,F(\rho_h^{(k)}) \;\le\; h\,F(\rho_h^{(k-1)})\,,$$

which may be summed over k to give

$$\sum_{k=1}^{N} \tfrac{1}{2\,h}\, d(\rho_h^{(k-1)}, \rho_h^{(k)})^2 \;+\; F(\rho_h^{(N)}) \;\le\; F(\rho^0)\,. \tag{46}$$

As in Proposition 4.1, we must confront the technical difficulty that F is not bounded below. The inequality (42) is established via the following calculations:

$$\begin{aligned}
M(\rho_h^{(N)}) &\overset{(17)}{\le} 2\,d(\rho^0, \rho_h^{(N)})^2 \;+\; 2\,M(\rho^0) \\
&\le\; 2\,N \sum_{k=1}^{N} d(\rho_h^{(k-1)}, \rho_h^{(k)})^2 \;+\; 2\,M(\rho^0) \\
&\overset{(46)}{\le} 4\,h\,N\,\Big(F(\rho^0) - F(\rho_h^{(N)})\Big) \;+\; 2\,M(\rho^0) \\
&\overset{(14)}{\le} 4\,T\,\Big(F(\rho^0) + C\,(M(\rho_h^{(N)}) + 1)^{\alpha}\Big) \;+\; 2\,M(\rho^0)\,,
\end{aligned}$$

which clearly gives (42). To obtain the second line of the above display, we have made use of the triangle inequality for the Wasserstein metric (see equation (9)) and the Cauchy–Schwarz inequality. The estimates (43), (44), and (45) now follow readily from the bounds (14) and (15), the estimate (42), and the inequality (46), as follows:

$$\begin{aligned}
\int_{R^n} \max\{\rho_h^{(N)}\, \log \rho_h^{(N)}, 0\}\, dx \;&\le\; S(\rho_h^{(N)}) \;+\; \int_{R^n} |\min\{\rho_h^{(N)}\, \log \rho_h^{(N)}, 0\}|\, dx \\
&\overset{(15)}{\le} S(\rho_h^{(N)}) \;+\; C\,(M(\rho_h^{(N)}) + 1)^{\alpha} \\
&\le\; F(\rho_h^{(N)}) \;+\; C\,(M(\rho_h^{(N)}) + 1)^{\alpha} \\
&\overset{(46)}{\le} F(\rho^0) \;+\; C\,(M(\rho_h^{(N)}) + 1)^{\alpha}\,;
\end{aligned}$$

$$\begin{aligned}
E(\rho_h^{(N)}) \;&=\; F(\rho_h^{(N)}) \;-\; S(\rho_h^{(N)}) \\
&\overset{(14)}{\le} F(\rho_h^{(N)}) \;+\; C\,(M(\rho_h^{(N)}) + 1)^{\alpha} \\
&\overset{(46)}{\le} F(\rho^0) \;+\; C\,(M(\rho_h^{(N)}) + 1)^{\alpha}\,;
\end{aligned}$$

$$\sum_{k=1}^{N} d(\rho_h^{(k-1)},\rho_h^{(k)})^2 \overset{(46)}{\leq} 2\,h\,\Big(F(\rho^0)\;-\;F(\rho_h^{(N)})\Big)$$
$$\overset{(14)}{\leq} 2\,h\,\Big(F(\rho^0)\;+\;C\,(M(\rho_h^{(N)})+1)^\alpha\Big)\,.$$

Now, owing to the estimates (42) and (43), we may conclude that there exists a measurable $\rho(t,x)$ such that, after extraction of a subsequence,

$$\rho_h \;\rightharpoonup\; \rho \quad \text{weakly in } L^1((0,T)\times\mathbb{R}^n) \quad \text{for all } T<\infty\,. \tag{47}$$

A straightforward analysis reveals that (42), (43), and (44) guarantee that

$$\begin{aligned} &\rho(t)\in K \quad \text{for a.e. } t\in(0,\infty)\,,\\ &M(\rho),\,E(\rho)\in L^\infty((0,T)) \quad \text{for all } T<\infty\,. \end{aligned} \tag{48}$$

Let us now improve upon the convergence in (47) by showing that (30) holds. For a given finite time horizon $T<\infty$, there exists a constant $C<\infty$ such that for all $N,N'\in\mathbb{N}$ and all $h\in[0,1]$ with $N\,h\leq T$, and $N'\,h\leq T$, we have

$$d(\rho_h^{(N')},\rho_h^{(N)})^2 \;\leq\; C\,|N'\,h-N\,h|\,.$$

This result is obtained from (45) by use of the triangle inequality (9) for d and the Cauchy–Schwarz inequality. Furthermore, for all $\rho,\rho'\in K\,,p\in\mathcal{P}(\rho,\rho')$, and $\zeta\in C_0^\infty(\mathbb{R}^n)$, there holds

$$\begin{aligned} \left|\int_{R^n}\zeta\,\rho'\,dx\;-\;\int_{R^n}\zeta\,\rho\,dx\right| &= \left|\int_{R^n\times R^n}(\zeta(x)\;-\;\zeta(y))\,p(dx\,dy)\right|\\ &\leq \sup_{R^n}|\nabla\zeta|\int_{R^n\times R^n}|x-y|\,p(dx\,dy)\\ &\leq \sup_{R^n}|\nabla\zeta|\left(\int_{R^n\times R^n}|x-y|^2\,p(dx\,dy)\right)^{\frac12}\,, \end{aligned}$$

so from the definition of d we obtain

$$\left|\int_{R^n}\zeta\,\rho'\,dx\;-\;\int_{R^n}\zeta\,\rho\,dx\right| \;\leq\; \sup_{R^n}|\nabla\zeta|\,d(\rho,\rho') \;\text{ for } \rho,\rho'\in K \text{ and } \zeta\in C_0^\infty(\mathbb{R}^n)\,.$$

Hence, it follows that

$$\left.\begin{aligned} &\left|\int_{R^n}\zeta\,\rho_h(t')\,dx\;-\;\int_{R^n}\zeta\,\rho_h(t)\,dx\right| \;\leq\; C\sup_{R^n}|\nabla\zeta|\;(|t'-t|+h)^{\frac12}\\ &\text{for all } t,t'\in(0,T),\ \text{and } \zeta\in C_0^\infty(\mathbb{R}^n)\,. \end{aligned}\right\} \tag{49}$$

Let $t\in(0,T)$ and $\zeta\in C_0^\infty(\mathbb{R}^n)$ be given, and notice that for any $\delta>0$, we have

$$\begin{aligned} &\left|\int_{R^n}\zeta\,\rho_h(t)\,dx\;-\;\int_{R^n}\zeta\,\rho(t)\,dx\right|\\ \leq\;& \left|\int_{R^n}\zeta\,\rho_h(t)\,dx\;-\;\tfrac{1}{2\,\delta}\int_{t-\delta}^{t+\delta}\int_{R^n}\zeta\,\rho_h(\tau)\,dx\,d\tau\right|\\ &+\left|\tfrac{1}{2\,\delta}\int_{t-\delta}^{t+\delta}\int_{R^n}\zeta\,\rho_h(\tau)\,dx\,d\tau\;-\;\tfrac{1}{2\,\delta}\int_{t-\delta}^{t+\delta}\int_{R^n}\zeta\,\rho(\tau)\,dx\,d\tau\right|\\ &+\left|\tfrac{1}{2\,\delta}\int_{t-\delta}^{t+\delta}\int_{R^n}\zeta\,\rho(\tau)\,dx\,d\tau\;-\;\int_{R^n}\zeta\,\rho(t)\,dx\right|\,. \end{aligned}$$

According to (49), the first term on the right-hand side of this equation is bounded by

$$C \sup_{R^n} |\nabla\zeta| \, (\delta + h)^{\frac{1}{2}} \,,$$

and owing to (47), the second term converges to zero as $h \downarrow 0$ for any fixed $\delta > 0$. At this point, let us remark that from the result (47) we may deduce that ρ is smooth on $(0,\infty)\times\mathbb{R}^n$. This is the conclusion of assertion (a) below, which will be proved later. From this smoothness property, we ascertain that the final term on the right-hand side of the above display converges to zero as $\delta \downarrow 0$. Therefore, we have established that

$$\int_{R^n} \zeta \, \rho_h(t) \, dx \;\to\; \int_{R^n} \zeta \, \rho(t) \, dx \quad \text{for all } \zeta \in C_0^\infty(\mathbb{R}^n) \,. \tag{50}$$

However, the estimate (42) guarantees that $M(\rho_h(t))$ is bounded for $h \downarrow 0$. Consequently, (50) holds for any $\zeta \in L^\infty(\mathbb{R}^n)$, and therefore, the convergence result (30) does indeed hold.

It now follows immediately from (41), (45), and (47) that ρ satisfies

$$\left.\begin{array}{l} -\displaystyle\int_{(0,\infty)\times R^n} \rho \, (\partial_t\zeta - \nabla\Psi\cdot\nabla\zeta + \Delta\zeta) \, dx \, dt \;=\; \int_{R^n} \rho^0 \, \zeta(0) \, dx \,, \\ \text{for all } \zeta \in C_0^\infty(\mathbb{R}\times\mathbb{R}^n) \,. \end{array}\right\} \tag{51}$$

In addition, we know that ρ satisfies (33). We now show that

(a) any solution of (51) is smooth on $(0,\infty)\times\mathbb{R}^n$ and satisfies equation (31);
(b) any solution of (51) for which (33) holds satisfies the initial condition (32);
(c) there is at most one smooth solution of (31) which satisfies (32) and (33).

The corresponding arguments are, for the most part, fairly classical.

Let us sketch the proof of the regularity part (a). First observe that (51) implies

$$\begin{aligned} \int_{R^n} \rho(t_1) \, \zeta(t_1) \, dx - \int_{(t_0,t_1)\times R^n} \rho \, (\partial_t\zeta - \nabla\Psi\cdot\nabla\zeta + \Delta\zeta) \; dx \; dt & \\ = \int_{R^n} \rho(t_0) \, \zeta(t_0) \, dx & \\ \text{for all } \; \zeta \in C_0^\infty(\mathbb{R}\times\mathbb{R}^n) \; \text{ and a.e. } \; 0 \le t_0 < t_1 \,. & \end{aligned} \tag{52}$$

We fix a function $\eta \in C_0^\infty(\mathbb{R}^n)$ to serve as a cutoff in the spatial variables. It then follows directly from (52) that for each $\zeta \in C_0^\infty(\mathbb{R}\times\mathbb{R}^n)$ and for almost every $0 \le t_0 < t_1$, there holds

$$\left.\begin{aligned} \int_{R^n} \eta \, \rho(t_1) \, \zeta(t_1) \, dx \;-\; & \int_{(t_0,t_1)\times R^n} \eta \, \rho \, (\partial_t\zeta + \Delta\zeta) \; dx \, dt \\ =\; & \int_{(t_0,t_1)\times R^n} \rho \; (\Delta\eta - \nabla\Psi\cdot\nabla\eta) \; \zeta \, dx \, dt \\ +\; & \int_{(t_0,t_1)\times R^n} \rho \; (2\,\nabla\eta - \eta\nabla\Psi)\cdot\nabla\zeta \, dx \, dt \\ +\; & \int_{R^n} \eta \, \rho(t_0) \, \zeta(t_0) \, dx \,. \end{aligned}\right\} \tag{53}$$

Notice that for fixed $(t_1, x_1) \in (0,\infty)\times\mathbb{R}^n$ and for each $\delta > 0$, the function

$$\zeta_\delta(t,x) \;=\; G(t_1 + \delta - t, x - x_1)$$

is an admissible test function in (53). Here G is the heat kernel

$$G(t,x) \;=\; t^{-\frac{n}{2}}\, g(t^{-\frac{1}{2}}x) \quad \text{with} \quad g(x) \;=\; (2\pi)^{-\frac{n}{2}} \exp(-\tfrac{1}{2}\,|x|^2). \tag{54}$$

Inserting ζ_δ into (53) and taking the limit $\delta \downarrow 0$, we obtain the equation

$$\left.\begin{aligned} (\rho\,\eta)(t_1) = & \int_{t_0}^{t_1} [\rho(t)\,(\Delta\eta - \nabla\Psi{\cdot}\nabla\eta)] * G(t_1-t)\,dt \\ + & \int_{t_0}^{t_1} [\rho(t)\,(2\,\nabla\eta - \eta\,\nabla\Psi)] * \nabla G(t_1-t)\,dt \\ & + (\rho\,\eta)(t_0) * G(t_1-t_0) \quad \text{for a.e. } 0 \le t_0 < t_1\,, \end{aligned}\right\} \tag{55}$$

where $*$ denotes convolution in the x-variables. From (55), we extract the following estimate in the L^p-norm:

$$\begin{aligned} \|(\rho\,\eta)(t_1)\|_{L^p} = & \int_{t_0}^{t_1} \|\rho(t)\,(\Delta\eta - \nabla\Psi{\cdot}\nabla\eta)\|_{L^1}\,\|G(t_1-t)\|_{L^p}\,dt \\ + & \int_{t_0}^{t_1} \|\rho(t)\,(2\,\nabla\eta - \eta\,\nabla\Psi)\|_{L^1}\,\|\nabla G(t_1-t)\|_{L^p}\,dt \\ & + \|(\rho\,\eta)(t_0)\|_{L^1}\,\|G(t_1-t_0)\|_{L^p} \quad \text{for a.e. } 0 \le t_0 < t_1\,. \end{aligned}$$

Now observe that

$$\begin{aligned} \|G(t)\|_{L^p} &= t^{(\frac{1}{p}-1)\,\frac{n}{2}}\,\|g\|_{L^p}\,, \\ \|\nabla G(t)\|_{L^p}, &= t^{\frac{1}{p}\,\frac{n}{2}-\frac{n+1}{2}}\,\|\nabla g\|_{L^p}\,, \end{aligned}$$

which leads to

$$\begin{aligned} & \|(\rho\,\eta)(t_1)\|_{L^p} \\ & = \ \operatorname*{ess\,sup}_{t\in(t_0,t_1)} \|\rho(t)\,(\Delta\eta - \nabla\Psi{\cdot}\nabla\eta)\|_{L^1} \int_0^{t_1-t_0} t^{(\frac{1}{p}-1)\,\frac{n}{2}}\,\|g\|_{L^p}\,dt \\ & \ + \operatorname*{ess\,sup}_{t\in(t_0,t_1)} \|\rho(t)\,(2\,\nabla\eta - \eta\,\nabla\Psi)\|_{L^1} \int_0^{t_1-t_0} t^{\frac{1}{p}\,\frac{n}{2}-\frac{n+1}{2}}\,\|\nabla g\|_{L^p}\,dt \\ & \ + \|(\rho\,\eta)(t_0)\|_{L^1}\,\|G(t_1-t_0)\|_{L^p} \quad \text{for a.e. } 0 \le t_0 < t_1\,. \end{aligned}$$

For $p < \frac{n}{n-1}$ the t-integrals are finite, from which we deduce that

$$\rho \;\in\; L^p_{\mathrm{loc}}((0,\infty){\times}\mathbb{R}^n)\,.$$

We now appeal to the L^p-estimates [18, section 3, (3.1), and (3.2)] for the potentials in (55) to conclude by the usual bootstrap arguments that any derivative of ρ is in $L^p_{\mathrm{loc}}((0,\infty){\times}\mathbb{R}^n)$, from which we obtain the stated regularity condition (a).

We now prove assertion (b). Using (55) with $t_0 = 0$, and proceeding as above, we obtain

$$\begin{aligned} & \|(\rho\,\eta)(t_1) \;-\; (\rho^0\,\eta) * G(t_1)\|_{L^1} \\ & = \ \operatorname*{ess\,sup}_{t\in(0,t_1)} \|\rho(t)\,(\Delta\eta - \nabla\Psi{\cdot}\nabla\eta)\|_{L^1} \int_0^{t_1} \|g\|_{L^1}\,dt \\ & \ + \operatorname*{ess\,sup}_{t\in(0,t_1)} \|\rho(t)\,(2\,\nabla\eta - \eta\,\nabla\Psi)\|_{L^1} \int_0^{t_1} t^{-\frac{1}{2}}\,\|\nabla g\|_{L^1}\,dt \quad \text{for all } t_1 > 0 \end{aligned}$$

and therefore,

$$(\rho\,\eta)(t) \;-\; (\rho^0\,\eta) * G(t) \;\to\; 0 \quad \text{in } L^1(\mathbb{R}^n) \quad \text{for } t \downarrow 0\,.$$

On the other hand, we have

$$(\rho^0\,\eta) * G(t) \;\to\; \rho^0\,\eta \quad \text{in } L^1(\mathbb{R}^n) \quad \text{for } t \downarrow 0\,,$$

which leads to

$$(\rho\,\eta)(t) \;\to\; \rho^0\,\eta \quad \text{in } L^1(\mathbb{R}^n) \quad \text{for } t \downarrow 0\,.$$

From this result, together with the boundedness of $\{M(\rho(t))\}_{t\downarrow 0}$, we infer that (32) is satisfied.

Finally, we prove the uniqueness result (c) using a well-known method from the theory of elliptic–parabolic equations (see, for instance, [20]). Let ρ_1, ρ_2 be solutions of (32) which are smooth on $(0,\infty)\times\mathbb{R}^n$ and satisfy (32), (33). Their difference ρ satisfies the equation

$$\frac{\partial \rho}{\partial t} \;-\; \operatorname{div}\left[\rho\,\nabla\Psi + \nabla\rho\right] \;=\; 0.$$

We multiply this equation for ρ by $\phi_\delta'(\rho)$, where the family $\{\phi_\delta\}_{\delta\downarrow 0}$ is a convex and smooth approximation to the modulus function. For example, we could take

$$\phi_\delta(z) \;=\; (z^2+\delta^2)^{\frac{1}{2}}\,.$$

This procedure yields the inequality

$$\begin{aligned}
&\partial_t[\phi_\delta(\rho)] \;-\; \operatorname{div}\left[\phi_\delta(\rho)\,\nabla\Psi + \nabla[\phi_\delta(\rho)]\right]\\
&= \;\; -\phi_\delta''(\rho)\,|\nabla\rho|^2 \;+\; (\phi_\delta'(\rho)\,\rho - \phi_\delta(\rho))\;\Delta\Psi\\
&\le \;\; (\phi_\delta'(\rho)\,\rho - \phi_\delta(\rho))\;\Delta\Psi,
\end{aligned}$$

which we then multiply by a nonnegative spatial cutoff function $\eta \in C_0^\infty(\mathbb{R}^n)$ and integrate over $\mathbb{R}^n$ to obtain

$$\begin{aligned}
\frac{d}{dt}\left[\int_{R^n} \phi_\delta(\rho(t))\,\eta\,dx\right] + \int_{R^n} \phi_\delta(\rho(t))\;(\nabla\Psi\cdot\nabla\eta - \Delta\eta)\;dx&\\
\le \int_{R^n} (\phi_\delta'(\rho)\,\rho - \phi_\delta(\rho))\;\Delta\Psi\,\eta\,dx\,.&
\end{aligned}$$

Integrating over $(0,t)$ for given $t \in (0,\infty)$, we obtain with help of (32)

$$\begin{aligned}
\int_{R^n} \phi_\delta(\rho(t))\,\eta\,dx \;+\; \int_{(0,t)\times R^n} \phi_\delta(\rho(t))\;(\nabla\Psi\cdot\nabla\eta - \Delta\eta)\;dx\,dt&\\
\le \int_{(0,t)\times R^n} (\phi_\delta'(\rho)\,\rho - \phi_\delta(\rho))\;\Delta\Psi\,\eta\,dx\,dt\,.&
\end{aligned}$$

Letting δ tend to zero yields

$$\int_{R^n} |\rho(t)|\,\eta\,dx \;+\; \int_{(0,t)\times R^n} |\rho(t)|\;(\nabla\Psi\cdot\nabla\eta - \Delta\eta)\;dx\,dt \;\le\; 0\,. \tag{56}$$

According to (12) and (33), ρ and $\rho\nabla\Psi$ are integrable on the entire $\mathbb{R}^n$. Hence, if we replace η in (56) by a function η_R satisfying

$$\eta_R(x) \;=\; \eta_1\left(\frac{x}{R}\right)\,, \quad \text{where } \;\eta_1(x) = 1 \;\text{ for } |x|\le 1\,,\;\; \eta_1(x) = 0 \;\text{ for } |x| \ge 2\,,$$

and let R tend to infinity, we obtain $\int_{R^n} |\rho(t)|\;dx = 0$. This produces the desired uniqueness result. ∎

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