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Sticky-reflecting diffusion as a Wasserstein gradient flow

Jean-Baptiste Casteras, Léonard Monsaingeon, Filippo Santambrogio

Abstract

In this paper we identify the Fokker-Planck equation for (reflected) Sticky Brownian Motion as a Wasserstein gradient flow in the space of probability measures. The driving functional is the relative entropy with respect to a non-standard reference measure, the sum of an absolutely continuous interior part plus a singular part supported on the boundary. Taking the small time-step limit in a minimizing movement (JKO scheme) we prove existence of weak solutions for the coupled system of PDEs satisfying in addition an Energy Dissipation Inequality.

1 Introduction

Since the work of R. Jordan, D. Kinderlehrer, and F. Otto [22] it is now well understood that the classical Fokker-Planck equation

$$\begin{cases} \partial_t \rho = \Delta \rho + \operatorname{div}(\rho \nabla V) & \text{in } \Omega \\ (\nabla \rho + \rho \nabla V) \cdot \nu = 0 & \text{on } \partial \Omega \end{cases}$$

can be reinterpreted as the Wasserstein gradient flow of the relative entropy in the space of probability measures

$$\frac{d\rho}{dt} = -\operatorname{grad}_{\mathcal{W}} \mathcal{H}(\rho|\mu),$$

where $\mu = \frac{1}{Z} e^{-V} \in \mathcal{P}(\Omega)$ is the stationary Gibbs measure associated with the background potential $V : \Omega \rightarrow \mathbb{R}$. Here \mathcal{W} is the quadratic Wasserstein distance over the smooth domain $\Omega \subset \mathbb{R}^d$, and $\mathcal{H}(\rho|\mu) = \int_{\Omega} \frac{\rho}{\mu} \log \left(\frac{\rho}{\mu} \right) d\mu$ is the relative entropy (Kullback-Leibler divergence) of ρ w.r.t. the reference measure μ . This has shed a whole new light on variational evolution of probability measures as gradient flows and the theory now covers advection-diffusion-aggregation equations [9, 5], Porous Medium Equation [31] and doubly nonlinear parabolic equations [1], fourth-order quantum drift-diffusion [27], reaction-diffusion equations with mass variations [24, 17, 12], and many more. We refer to the by-now classical textbooks [38, 37, 34] as well as to the survey [35] for further discussions, references, and applications of this steadily growing topics.

A common feature of all the aforementioned models and equations is that they deal with measures $\rho = \rho(x) \cdot dx$ which are absolutely continuous with respect to either the Lebesgue measure in Euclidean domains, or its equivalent - the volume form - in Riemannian manifolds. For the standard Fokker-Planck equation this is clearly legitimate due to strong regularizing properties of the Laplacian, the generator of the standard (reflected) Brownian Motion with stationary measure precisely given by the Lebesgue measure. Recently however, the so-called (reflected) *Sticky Brownian Motion* [15] (SBM in short) started attracting renewed interest [33, 13, 7, 23]. Roughly speaking, SBM is a \mathbb{R}^d -valued stochastic process which behaves as a standard diffusion as long as it remains in the interior of a prescribed domain $\Omega \subset \mathbb{R}^d$. When it hits the boundary $\Gamma = \partial \Omega$ it sticks there for a random positive amount of time, while following an intrinsic tangential diffusion (generated by the Laplace-Beltrami operator Δ_{Γ} thereon). Eventually SBM almost surely reenters the domain and resumes its standard Brownian behaviour, until hitting the boundary again, and so on. We refer to [20, 14] for the

construction and regularity properties of SBM via Dirichlet-forms. In functional analytic terms, SBM is best described by its generator

$$\mathcal{L}f(x) = \lim_{t \downarrow 0} \frac{\mathbb{E}f(X_t) - f(x)}{t} = \begin{cases} \frac{1}{2}\Delta f(x) & \text{if } x \in \Omega \\ \frac{a}{2}\Delta_\Gamma f(x) - b\partial_\nu f(x) & \text{if } x \in \Gamma = \partial\Omega \end{cases}$$

where the parameters $a, b > 0$ are the tangential diffusivity and stickiness of the SBM process, respectively. The stationary measure accordingly comprises an interior \mathcal{L}_Ω^d and boundary \mathcal{L}_Γ^{d-1} Lebesgue measures, and the laws of motion couple the interior domain and its boundary through an exchange term. The relevant probability distributions thus cannot simply be absolutely continuous, and we write throughout

$$\rho = \omega + \gamma \in \mathcal{P}(\overline{\Omega}) \quad \text{with} \quad \begin{cases} \omega = \rho \llcorner \Omega \in \mathcal{M}^+(\Omega) \\ \text{and} \\ \gamma = \rho \llcorner \Gamma \in \mathcal{M}^+(\Gamma) \end{cases}$$

for the associated interior/boundary decomposition $\overline{\Omega} = \Omega \cup \Gamma$. Discarding the probabilistic $\frac{1}{2}$ factors for convenience, the abstract Fokker-Planck equation $\partial_t \rho = \mathcal{L}^* \rho$ for pure SBM reads here

$$\begin{cases} \partial_t \omega = \Delta \omega & \text{in } \Omega \\ \omega = b\gamma & \text{on } \partial\Omega. \\ \partial_t \gamma = a\Delta_\Gamma \gamma - \partial_\nu \omega & \text{in } \Gamma \end{cases} \quad (1.1)$$

In terms of PDEs this is a coupled system of bulk/interface diffusions, and the $\partial_\nu \omega$ exchange term corresponds at the stochastic level to the jump rate between the two interior/boundary behaviours. Here we focus on the case $a = b = 1$, and in this paper we shall make a case that this is again a gradient flow

$$\begin{cases} \partial_t \omega = \Delta \omega & \text{in } \Omega \\ \omega = \gamma & \text{on } \partial\Omega \\ \partial_t \gamma = \Delta_\Gamma \gamma - \partial_\nu \omega & \text{in } \Gamma \end{cases} \Leftrightarrow \frac{d\rho}{dt} = -\text{grad}_{\mathcal{W}} \mathcal{H}(\rho | \mu) \quad \text{for } \mu := \mathcal{L}_\Omega^d + \mathcal{L}_\Gamma^{d-1}. \quad (1.2)$$

Perhaps surprisingly, the transportation distance involved here is still the classical, quadratic Wasserstein distance \mathcal{W} over $\overline{\Omega}$. This is due to our crucial assumption that $a = 1$, for which the interior Δ and boundary Δ_Γ diffusions are tangentially matched. For $a \neq 1$ the transportation distance must be adapted and the analysis is quite different. This will be investigated in a future work [10]. The case of coefficients $b \neq 1$ can however be treated by simply adapting the reference measure $\mu_b = b\mathcal{L}_\Omega^d + \mathcal{L}_\Gamma^{d-1}$ in the driving functional $\rho \mapsto \mathcal{H}(\rho | \mu_b)$, and we chose to focus on $b = 1$ only to clarify the exposition. Similarly, background potentials V_Ω, V_Γ could very well be included in the total free energy $\mathcal{F} = \mathcal{H} + \int_\Omega V_\Omega d\omega + \int_\Gamma V_\Gamma d\gamma$ in order to account for drift in the Fokker-Planck equation, but we simply ignore this possibility in order not to overburden the analysis. Note that a rather complete mathematical analysis (existence, uniqueness, regularity) of (1.1) has been carried out in [36] within a $H^1(\Omega) \times H^1(\Gamma)$ functional framework. For the smooth, positive solutions constructed therein, integration by parts gives

$$\begin{aligned} \frac{d}{dt} \mathcal{H}(\rho_t | \mu) &= \frac{d}{dt} \left(\int_\Omega \omega_t \log \omega_t + \int_\Gamma \gamma_t \log \gamma_t \right) \\ &= \int_\Omega (1 + \log \omega_t) \Delta \omega_t + \int_\Gamma (1 + \log \gamma_t) [\Delta_\Gamma \gamma_t - \partial_\nu \omega_t] \\ &= \left[- \int_\Omega |\nabla \log \omega_t|^2 \omega_t + \int_{\partial\Omega} (1 + \log \omega_t) \partial_\nu \omega_t \right] \\ &\quad + \left[- \int_\Gamma |\nabla_\Gamma \log \gamma_t|^2 \gamma_t - \int_\Gamma (1 + \log \gamma_t) \partial_\nu \omega_t \right] \\ &= - \int_\Omega |\nabla \log \omega_t|^2 \omega_t - \int_\Gamma |\nabla_\Gamma \log \gamma_t|^2 \gamma_t =: -\mathcal{I}(\omega_t) - \mathcal{I}(\gamma_t). \quad (1.3) \end{aligned}$$

In the last equality we used the Dirichlet boundary condition $\omega_t|_{\partial\Omega} = \gamma_t$ to cancel out the boundary terms (more on this in a moment). This shows that the relative entropy $\mathcal{H}(\rho|\mu) = \int_{\Omega} \omega \log \omega + \int_{\Gamma} \gamma \log \gamma$ of $\rho = \omega + \gamma$ is dissipated by the sum of the full Fisher information $\mathcal{I}(\omega)$ inside Ω and the tangential Fisher information $\mathcal{I}(\gamma)$ along the boundary $\Gamma = \partial\Omega$. Here our focus is not really on the well-posedness (although our analysis will provide as a byproduct existence of weak solutions for initial data with merely finite entropy), and we rather take interest in the variational gradient flow structure underlying this dissipation relation.

Although one can certainly come up with models naturally taking into account bulk/interface interactions directly into the transportation distance [30, 19], we find surprising that the coupled system (1.2) still fits within a completely standard optimal transport framework, as far as the metric is concerned. Another striking aspect of our analysis is the following: For standard Fokker-Planck equations the usual no-flux boundary condition encodes local conservation of mass, while in (1.2) one may wonder where the boundary condition $\omega|_{\partial\Omega} = \gamma$ stems from (this trace compatibility was crucial in order to get to (1.3)). This is actually unrelated to mass conservation: Our two evolution equations for ω, γ put together are already mass conservative regardless of the extra boundary condition $\omega|_{\partial\Omega} = \gamma$, since $\partial_\nu \omega$ in the second PDE is precisely the outflux of the momentum $\nabla \omega$ appearing in the first one so whatever “comes out of Ω ” is just transferred to the boundary (the two PDEs together can indeed be reinterpreted as a single continuity equation $\partial_t \rho + \operatorname{div} m = 0$ with no-flux condition for the total density $\rho = \omega + \gamma$, but with a singular part γ living on the boundary in addition to a usual absolutely continuous part ω in the interior). The Dirichlet boundary condition $\omega|_{\partial\Omega} = \gamma$ is also not merely encoded as a constraint in the entropy functional itself, since finiteness of $\mathcal{H}(\rho|\mu)$ certainly does not require or guarantee the trace compatibility. For the sake of completeness let us mention that in [16] a transportation distance was constructed on $\mathcal{M}^+(\Omega)$, using the boundary $\Gamma = \partial\Omega$ as an infinite reservoir allowing to store and release arbitrary amounts of mass. It was then showed that the gradient flow of the standard entropy (with dx as a reference measure) with respect to this new distance corresponds to the heat equation with Dirichlet boundary condition $\rho|_{\partial\Omega} = 1$. Although similar in spirit this is actually unrelated to our approach here, since our model is really mass conservative in all regards. As we shall see later on, our boundary condition rather arises from the energy-dissipation mechanism, and more precisely from the *metric slope* of the driving functional (see Theorem 1). To the best of our knowledge this is the first example of an optimal transport model in which entropy dissipation (rather than entropy itself) gives rise to Dirichlet boundary conditions. In order to illustrate this even further, one could consider different energies, for example of the form

$$\mathcal{F}(\rho) = \int_{\Omega} F_{\Omega}(\omega) dx + \int_{\Gamma} F_{\Gamma}(\gamma) dx, \quad \rho = \omega + \gamma$$

for some functions $F_{\Omega}, F_{\Gamma} : \mathbb{R}^+ \rightarrow \mathbb{R}$ satisfying suitable structural conditions. The gradient flow would then read

$$\frac{d\rho}{dt} = -\operatorname{grad}_{\mathcal{W}} \mathcal{F}(\rho) \quad \Leftrightarrow \quad \begin{cases} \partial_t \omega = \operatorname{div}(\omega \nabla F'_{\Omega}(\omega)) & \text{in } \Omega \\ F'_{\Omega}(\omega)|_{\partial\Omega} = F'_{\Gamma}(\gamma) & \text{on } \partial\Omega \\ \partial_t \gamma = \operatorname{div}_{\Gamma}(\gamma \nabla_{\Gamma} F'_{\Gamma}(\gamma)) - \omega \partial_{\nu} F'_{\Omega}(\omega) & \text{in } \Gamma. \end{cases}$$

The scalar fields $F'_{\Omega}(\omega), F'_{\Gamma}(\gamma)$ are known in classical optimal transport as *pressure variables* (in this respect the two evolution equations are nothing but Darcy’s law). Very heuristically, a pressure difference along Γ would create somehow an infinite force. From a variational standpoint this should be prohibited for dissipative systems. Thus the Dirichlet boundary condition can be reinterpreted as a dissipative, pressure matching condition.

On a slightly different note, the theory of gradient flows in abstract metric spaces and *curves of maximal slope* was initiated by De Giorgi [11], and more recently developed in [2]. One possible way of formalizing the notion of such abstract gradient flows is to prove convergence of De Giorgi’s *minimizing movement* in the small time-step limit $\tau \rightarrow 0$, of which the original JKO

scheme [22] is a particular instantiation in the Wasserstein space $(\mathcal{P}(\Omega), \mathcal{W})$. In order to back-up our claim (1.2) that sticky diffusion is indeed a gradient flow we will pursue this by now classical approach, with however a few twists. First, there are two classical ways of proving that the limiting curve is a “solution”. The first one consists in exploiting purely metric tools to retrieve in the limit an *Energy Dissipation Inequality* (EDI in short), where a dissipation functional $\mathcal{D}(\rho_t) = -\frac{d}{dt}\mathcal{E}(\rho_t)$ plays a key role together with the *metric speed* $|\dot{\rho}_t|^2$ (both computed with respect to the Wasserstein distance). Usually the dissipation is related to the *metric slope* $\mathcal{D}(\rho) = |\partial\mathcal{E}|^2(\rho)$, typically a Fisher information functional $\mathcal{I}(\rho)$, and this guarantees that the limit is a curve of maximal slope. Moreover an upper chain rule argument shows that the energy dissipation forces equality in a Cauchy-Schwarz inequality, thus relating the driving momentum m in the continuity equation $\partial_t\rho + \operatorname{div} m = 0$ to spatial gradients of the energy $m = -\rho\nabla\frac{\delta\mathcal{E}}{\delta\rho}$. This gives the PDE in the end, but really requires a chain rule (computing the derivative in time of the energy \mathcal{E} along a curve). This is well understood for classical functionals [2, chapter 10], less so here, and we did not fully succeed in this respect (see Theorem 1 and our Conjecture 2).

The second classical approach is directly PDE-oriented and less related to dissipation: Leveraging ad-hoc tools from optimal transportation theory, one usually writes down the discrete Euler-Lagrange optimality condition for each step $\rho^n \rightsquigarrow \rho^{n+1}$ of the JKO scheme, and tries passing to the limit $\tau \rightarrow 0$ to retrieve the continuous PDE directly from the one-step optimality. In the classical Fokker-Planck case this strongly relies on the Brenier-McCann theorem [8, 29], allowing to relate the optimal map in $\rho^{n+1} = T^n\#\rho^n$ with the energy. More precisely, the Euler-Lagrange equation $\frac{T^n(x)-x}{\tau} = -\nabla\frac{\delta\mathcal{E}}{\delta\rho}(\rho^{n+1})$ typically gives the discrete velocity field driving particles around in the end (displacement $T^n(x) - x$ divided by time τ). This technical tool is unfortunately not available here, since our entropy functional always forces $\rho^n = \omega^n + \gamma^n$ to have a singular part γ^n supported on the boundary and therefore systematically prevents any application of the Brenier-McCann theorem (which precisely requires ρ not to give mass to small \mathcal{H}^{d-1} sets in dimension d !). In some sense the bulk-interface interaction, corresponding to the $\partial_\nu\omega$ exchange term in (1.2), forces mass splitting already at the discrete level. In order to circumvent this technical obstacle and still obtain a useful Euler-Lagrange equation we perform instead an ad-hoc ε -regularization of the entropy functional, and show that the barycentric momentum conveys enough information in order to first pass to the limit $\varepsilon \rightarrow 0$ and then take $\tau \rightarrow 0$.

Let us now fix some notations. We always work in a smooth, bounded, convex domain $\Omega \subset \mathbb{R}^d$, $d \geq 2$. (We assume convexity for technical convenience only, but the result should hold for general domains.) We set

$$H(z) := z \log z - z + 1 \geq 0, \quad z \geq 0,$$

and the reference measure will always be

$$\mu := \mathcal{L}_\Omega^d + \mathcal{L}_\Gamma^{d-1} \in \mathcal{M}^+(\overline{\Omega}).$$

The entropy

$$\mathcal{E}(\rho) := \mathcal{H}(\rho|\mu) = \begin{cases} \int_\Omega H\left(\frac{d\rho}{d\mu}(x)\right) \mu(dx) & \text{if } \rho \ll \mu \\ +\infty & \text{else} \end{cases} \quad (1.4)$$

is then nonnegative, strictly convex, and lower semi-continuous. As suggested by (1.3) we define the dissipation

$$\mathcal{D}(\rho) := \begin{cases} \mathcal{I}(\omega) + \mathcal{I}(\gamma) & \text{if } \rho = \omega + \gamma \text{ and } \omega|_{\partial\Omega} = \gamma \\ +\infty & \text{else} \end{cases} \quad (1.5)$$

(see later on for a rigorous definition of the Fisher information functional \mathcal{I} as well as the precise meaning of the boundary trace $\omega|_{\partial\Omega}$). This penalization of the constraint $\omega|_{\partial\Omega} = \gamma$ is not technically artificial and arises intrinsically when trying to compute the metric slope $|\partial\mathcal{E}|$, see Theorem 1 below.

Given an initial datum $\rho_0 \in \mathcal{P}(\overline{\Omega})$, the JKO scheme consists in initializing $\rho^0 = \rho_0$ and solving recursively

$$\rho^{n+1} \in \operatorname{Argmin}_{\rho \in \mathcal{P}(\overline{\Omega})} \left\{ \frac{1}{2\tau} \mathcal{W}^2(\rho, \rho^n) + \mathcal{E}(\rho) \right\}. \quad (1.6)$$

With such a discrete sequence one can define the piecewise constant interpolation

$$\overline{\rho}_t^\tau := \rho^{n+1} \quad \text{for} \quad t \in (n\tau, (n+1)\tau],$$

and we will establish

Main result. *Fix any $\rho_0 \in \mathcal{P}(\overline{\Omega})$ with $\mathcal{E}(\rho_0) < \infty$. For any small $\tau > 0$ the JKO scheme (1.6) is uniquely well-posed, and there is a discrete sequence $\tau \rightarrow 0$ such that the interpolant $\overline{\rho}^\tau$ converges to a continuous curve $\rho : [0, \infty) \rightarrow \mathcal{P}(\overline{\Omega})$*

$$\mathcal{W}(\overline{\rho}_t^\tau, \rho_t) \xrightarrow{\tau \rightarrow 0} 0 \quad \text{for all } t \geq 0.$$

The limit satisfies the Energy Dissipation Inequality

$$\mathcal{E}(\rho_T) + \int_0^T \left(\frac{1}{2} |\dot{\rho}_t|^2 + \frac{1}{2} \mathcal{D}(\rho_t) \right) dt \leq \mathcal{E}(\rho_0), \quad \forall T > 0$$

and is a weak solution of the PDE (1.2). Moreover, there is $\lambda > 0$ only depending on Ω such that

$$\mathcal{H}(\rho_t | \bar{\mu}) \leq e^{-2\lambda t} \mathcal{H}(\rho_0 | \bar{\mu}) \quad \text{and} \quad |\rho_t - \bar{\mu}|_{TV} \leq e^{-\lambda t} \sqrt{\frac{1}{2} \mathcal{H}(\rho_0 | \bar{\mu})}, \quad \forall t \geq 0 \quad (1.7)$$

where $\bar{\mu} := \frac{1}{\mu(\overline{\Omega})} \mu$ is the renormalized stationary measure. Finally, if $\rho_0 \leq \bar{c} \mu$ for some constant $\bar{c} > 0$ (resp. $\rho_0 \geq \underline{c} \mu$ for some \underline{c}) then $\rho_t \leq \bar{c} \mu$ for all $t \geq 0$ (resp. $\rho_t \geq \underline{c} \mu$).

It is worth stressing that something is still missing in order to obtain a rigorous metric gradient flow. Indeed, in order for EDI to fully characterize curves of maximal slope one should really prove that $g(\rho) = \sqrt{\mathcal{D}(\rho)}$ is an *upper gradient* [2, chapter 1]. The local slope $|\partial \mathcal{E}|$ is always a (weak) upper gradient, and we conjecture that $\mathcal{D} = |\partial \mathcal{E}|^2$ thus it is plausible that $\sqrt{\mathcal{D}}$ should be an upper gradient. However we only managed to prove that $\mathcal{D} \leq |\partial \mathcal{E}|^2$, and we were also not able to prove directly that $\sqrt{\mathcal{D}}$ is an upper gradient.

Another key concept for the abstract theory of metric gradient flows is that of geodesic convexity, or, in the specific optimal transport framework, McCann's displacement convexity [28]. In smooth, complete Riemannian manifolds the λ -convexity of \mathcal{H} (relatively to the reference volume measure) is equivalent to λ -Ricci lower bounds. In Euclidean domains, it is known to hold with $\lambda = 0$ if and only if Ω is convex, which can also be reinterpreted as the fact that the subspace $\mathcal{P}_{\mathcal{L}_\Omega^{ac}}(\overline{\Omega}) \subset \mathcal{P}(\overline{\Omega})$ of absolutely continuous measures (w.r.t. to the reference Lebesgue measure \mathcal{L}_Ω^d) is geodesically convex. It is worth stressing that this whole picture collapses here: Due to our choice of reference measure $\mu = \mathcal{L}_\Omega^d + \mathcal{L}_\Gamma^{d-1}$ the entropy $\mathcal{E}(\rho) = \mathcal{H}(\rho | \mu)$ cannot be λ -convex for any $\lambda \in \mathbb{R}$, even if the underlying domain Ω is strongly uniformly convex. This is due to the fact that $\mathcal{P}_\mu^{ac}(\overline{\Omega})$ itself fails to be geodesically convex. For a counterexample, take Ω the unit ball, and consider two measures $\rho_0 = 0 + \gamma_0, \rho_1 = 0 + \gamma_1$ smoothly supported on the boundary as in Figure 1, with finite entropies $\mathcal{E}(\rho_i) = \mathcal{H}(\gamma_i | \mathcal{L}_\Gamma^{d-1}) < \infty$. It is not difficult in this configuration to check that the unique geodesic ρ_t remains singular (and absolutely continuous w.r.t. \mathcal{H}^{d-1}) and supported strictly inside Ω for all intermediate times $t \in (0, 1)$. As a consequence $\rho_t = \omega_t + 0$ is not absolutely continuous w.r.t. μ and thus $\mathcal{E}(\rho_t) = +\infty$ for all $t \in (0, 1)$, while $\mathcal{E}(\rho_0), \mathcal{E}(\rho_1) < +\infty$.

It is also known that geodesic convexity usually leads to logarithmic Sobolev and entropy-entropy production inequalities, which in turn should yield exponential convergence as $t \rightarrow \infty$ towards the unique entropy minimizer, here $\bar{\mu} = \frac{1}{|\Omega| + |\Gamma|} \mu \in \mathcal{P}(\overline{\Omega})$. Although convexity completely fails here as just discussed, it was proved nonetheless in [6] that $\bar{\mu}$ always satisfies a