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Stochastic differential equations on domains defined by multiple constraints

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Abstract

We present simple assumptions on the constraints defining a hard core dynamics for the associated reflected stochastic differential equation to have a unique strong solution. Time-reversibility is proven for gradient systems with normal or co-normal reflection. An illustration is given concerning the clustering at equilibrium of particles around a large attractive sphere.

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1 Introduction

Since the first works of Skorokhod [14] on existence and uniqueness for pathwize solutions of reflected stochastic differential equations, many authors have investigated this type of equation and extended his results on half-spaces to more general domains: convex sets (Tanaka [15]), admissible sets (Lions-Sznitman [8]), domains satisfying only the Uniform Exterior Sphere and the Uniform Normal Cone conditions (Saisho [10]), or some weaker version of these conditions (Dupuis and Ishii [4]). The question of equilibrium states of the reflected process (construction of time-reversible initial measures) has also been investigated (see e.g. [13]).

All these studies were done under some smoothness assumptions on the boundary of the domain. Typically the existence of at least one normal inward vector at each point of the boundary is a necessary condition to define the normal reflection direction.

In most cases, the domain in which the process has to live is defined by constraints which are physically natural rather than by its geometrical properties as a subset of some Euclidean space. For example consider a system of n identical hard spheres with radius r in $\mathbb{R}^d$. The domain in which they evolve is the set of configurations $(x_i)_{1\le i\le n}$ satisfying the constraints $|x_i - x_j| > 2r$ (i.e. the distance between the centers of any two spheres is larger than twice their radius). The geometrical description is much more complicated: the complementary set in $\mathbb{R}^{nd}$ of some star-convex subset whose boundary can be locally approximated by a tangent sphere and a cone.

Unfortunately, for reflected processes in dimension larger than three, the geometrical properties of the domain are not that obvious from the physical constraints. In the already mentioned nd-dimensional example of a finite system of hard spheres, the paper [11] mainly consists in the proof that the set of allowed ball configurations satisfies

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the Uniform Exterior Sphere and Uniform Interior Cone property. In [12] and [5] too, a meticulous and extensive geometrical study has to be performed before the stochastic analysis of the dynamics.

We present in this note a constraint-based assumption to construct pathwise solutions of Skorokhod problems (even for non-reversible dynamics). Our aim is to deal with assumptions as simple and physically natural as possible, even if they are not the weakest ones.

In the special case of time-reversible dynamics, Skorokhod problems can be studied using potentiel theory. This Dirichlet form approach allows constructions on relatively non-smooth domains, as done in the seminal article of Chen [3]. But our aim here is to deal with either reversible or non-reversible cases. We want an explicit criterion on the constraints which enables a pathwise construction of the solution, i.e. it constructs the path $\mathbf{X}$ and its local time $\mathbf{L}$ as a function of the path $\mathbf{W}$ of the Brownian motion defined on the underlying Probability space. So the technics are closer to Saisho's approach than to potentiel theory.

This note is divided in two parts.

The first part (section 2) exhibits a new compatibility criterion for constraints. If it is satisfied, then the reflected stochastic differential equation admits a unique strong solution. The proof uses the Uniform Exterior Sphere and the Uniform Normal Cone conditions, hence it ultimately relies on the convergence of the discretized Brownian pathes projected on the subset of $\mathbb{R}^d$ where all the constraints are satisfied. The solution is time-reversible in the special case of a gradient system whose reflection direction is consistent with its diffusion coefficient.

In section 3 we present an illustration inspired by [2]. We consider the behaviour of many spherical particles around a sphere. They are submitted to a smooth attractive influence and their motion is perturbated by collisions into other particles and into the sphere. We prove that at equilibrium and for low temperature all particles are as close as possible, all located beneath some altitude with high probability. Applications to more realistic models (see e.g. [9] or [1]) are currently investigated.

2 Reflected stochastic differential equation under multiple constraints

We are interested in a process living in the closure of a domain $\mathcal{D}$. This domain is defined by a finite set $\mathcal{F}$ of smooth $\mathbb{R}$-valued constraint functions on $\mathbb{R}^d$:

$$\mathcal{D} = \left\{ \mathbf{x} \in \mathbb{R}^d;\ f(\mathbf{x}) > 0 \text{ for each } f \in \mathcal{F} \right\}.$$

$\mathcal{D}$ is an intersection of smooth sets (arbitrary many of them provided they are in finite number) so its boundary is a finite union of smooth boundaries:

$$\partial\mathcal{D} = \bigcup_{f\in\mathcal{F}} \left\{ \mathbf{x} \in \overline{\mathcal{D}};\ f(\mathbf{x}) = 0 \right\}.$$

Since we want the process to be reflected on the boundary of $\mathcal{D}$ we have to assume some regularity on the functions in $\mathcal{F}$. The reflection at any point $\mathbf{x} \in \partial\mathcal{D}$ occurs either in the inward normal direction $\nabla f(\mathbf{x})$ or with a fixed deviation from the normal direction. So we have to suppose the existence of a direction which is normal to the boundary: $\nabla f(\mathbf{x}) \neq 0$ for each $\mathbf{x} \in \overline{\mathcal{D}}$ such that $f(\mathbf{x}) = 0$. We actually assume something more: the first derivative of the functions of $\mathcal{F}$ admits some positive uniform lower bound, their second derivative is uniformly bounded and, most important, the boundary of each single-constraint set $\{\mathbf{x}\ ;\ f(\mathbf{x}) > 0\}$ crosses the boundaries of the other single-constraint sets at "not too sharp an angle". To be more precise, we have to exclude infinitely sharp "thorns" whose vertex admits inward normal vectors in opposite directions. This is what we call *compatibility* between the constraints:

Definition 2.1. *Let $\mathcal{F}$ be a finite set of $\mathbb{R}$-valued $\mathcal{C}^2$-functions on $\mathbb{R}^d$. These functions are called* compatible constraints *if*

- $\mathcal{D} := \left\{\mathbf{x} \in \mathbb{R}^d;\ f(\mathbf{x}) > 0 \text{ for each } f \in \mathcal{F}\right\}$ *is a non-empty connected set ;*
- *for each* $f \in \mathcal{F}$, $\inf\{|\nabla f(\mathbf{x})|;\ \mathbf{x} \in \overline{\mathcal{D}},\ f(\mathbf{x}) = 0\} > 0$ *and* $\sup\{|D^2 f(\mathbf{x})|;\ \mathbf{x} \in \mathbb{R}^d\} < +\infty$ *;*
- $\inf_{\mathbf{x}\in\partial\mathcal{D}} \delta(0, \mathrm{Conv}(\mathbf{x})) > 0$
  where $\mathrm{Conv}(\mathbf{x})$ *is the convex hull of the unit normal vectors to the boundaries at point* $\mathbf{x}$*:*

$$\mathrm{Conv}(\mathbf{x}) = \left\{ \sum_{f\in\mathcal{F}, f(\mathbf{x})=0} c_f \frac{\nabla f(\mathbf{x})}{|\nabla f(\mathbf{x})|} \quad \textit{s.t.} \quad c_f \geq 0 \textit{ and} \sum_{f\in\mathcal{F}, f(\mathbf{x})=0} c_f = 1 \right\}.$$

Here and in the sequel, δ denotes the Euclidean distance in $\mathbb{R}^d$, $|\mathbf{y}|$ denotes the Euclidean norm of vector $\mathbf{y}$ and $|M| = \sup\{|M\mathbf{y}|/|\mathbf{y}|\ ;\ \mathbf{y} \in \mathbb{R}^d\}$ denotes the norm of the matrix M. Lebesgue measure is denoted by $d\mathbf{x}$.

The next main theorem states that our compatibility definition provides a convenient assumption to ensure the existence of a reflected process within a set defined by constraints. In most models, for the sake of simplicity, the reflection direction is the inward *normal* direction on the boundary. Here we consider a *co-normal* reflection, as in the case treated in [6] or in Section 3. We state the result with a fixed deviation $\boldsymbol{\theta}\ {}^t\boldsymbol{\theta}$ from the normal direction. ${}^t\boldsymbol{\theta}$ denotes the transposed matrix. Normal reflection corresponds to the special case $\boldsymbol{\theta} = I_d$.

Theorem 2.2 (Existence and uniqueness)**.** *Let $\boldsymbol{\theta}$ be a fixed $d \times d$ invertible matrix and $\mathcal{F}$ be a set of compatible constraints with $\mathcal{D} = \bigcap_{f\in\mathcal{F}} \left\{\mathbf{x} \in \mathbb{R}^d;\ f(\mathbf{x}) > 0\right\}$ the corresponding subset of $\mathbb{R}^d$. If $\boldsymbol{\sigma} : \overline{\mathcal{D}} \longrightarrow \mathbb{R}^{d^2}$ and $\mathbf{b} : \overline{\mathcal{D}} \longrightarrow \mathbb{R}^d$ are bounded Lipschitz continuous functions on $\overline{\mathcal{D}}$, then the reflected stochastic differential equation*

$$\mathbf{X}(t) = \mathbf{x} + \int_0^t \boldsymbol{\sigma}(\mathbf{X}(s))d\mathbf{W}(s) + \int_0^t \mathbf{b}(\mathbf{X}(s))ds + \sum_{f\in\mathcal{F}} \int_0^t \boldsymbol{\theta}\ {}^t\boldsymbol{\theta} \nabla f(\mathbf{X}(s))dL_f(s) \tag{2.1}$$

has for each starting point $\mathbf{x} \in \mathcal{D}$ a unique strong solution in $\overline{\mathcal{D}}$, where the local times L_f satisfy $L_f(\cdot) = \int_0^{\cdot} \mathbb{1}_{f(\mathbf{X}(s))=0}\ dL_f(s)$.

In this theorem "strong uniqueness of the solution" stands for strong uniqueness in the sense of [7] chap.IV def.1.6 of the process $\mathbf{X}$, not of the local times L_f.

Lemma 2.3. *In definition 2.1 the condition $\inf_{\mathbf{x}\in\partial\mathcal{D}} \delta(0, \mathrm{Conv}) > 0$ is equivalent to*

$$\exists\beta_0 > 0 \quad \forall\mathbf{x} \in \partial\mathcal{D} \quad \exists\mathbf{v} \neq 0 \quad \forall f \in \mathcal{F} \textit{ s.t. } f(\mathbf{x}) = 0 \quad \mathbf{v}.\nabla f(\mathbf{x}) \geq \beta_0|\mathbf{v}|\ |\nabla f(\mathbf{x})|$$

where the dot denotes the Euclidean scalar product.

Though this statement is longer and apparently more difficult to obtain than an uniform lower bound on the norms of the convex combinations, it is in some sense more intuitive. It states the existence of cones (with vertex $\mathbf{x}$, axis $\mathbf{v}$ and aperture $2\arccos\beta_0$) which contain all the inward normal vectors given by the constraints at point $\mathbf{x}$. The positivity condition ensures that these cones do not degenerate into half-spaces. This condition is easier to check in some concrete situations (e.g. section 3).

Lemma 2.4 (Stability of the compatibility property)**.** *Let $\mathcal{F}$ be a set of compatible constraints on $\mathbb{R}^d$.*

- *If $\boldsymbol{\theta}$ is a $d \times d$ invertible matrix, the transformed constraints $\{f(\boldsymbol{\theta}\ \cdot);\ f \in \mathcal{F}\}$ are compatible.*
- *If all constraints disregard one of the coordinates then $\mathcal{F}$ induces a set of compatible constraints on $\mathbb{R}^{d-1}$, that is, if $f(x_1, \cdots, x_{d-1}, x_d) = f(x_1, \cdots, x_{d-1}, 0)$ for each f in $\mathcal{F}$ and each $\mathbf{x} = (x_1, \cdots, x_d)$ in $\mathbb{R}^d$ then $\left\{ \underline{f} : \begin{array}{l} \mathbb{R}^{d-1} \longrightarrow \mathbb{R} \\ \underline{\mathbf{x}} \longmapsto f(\underline{\mathbf{x}}, 0) \end{array} ;\ f \in \mathcal{F} \right\}$ is compatible.*

In the special case where $\boldsymbol{\sigma}$ is constant and $\mathbf{b}$ is a gradient, equation (2.1) admits a time-reversible measure μ (i.e. the distribution of the solution with initial measure μ is invariant under the transformation $\big(\mathbf{X}(\cdot), (L_f(\cdot))_{f\in\mathcal{F}}\big) \longrightarrow \big(\mathbf{X}(T-\cdot), (L_f(T-\cdot) - L_f(T))_{f\in\mathcal{F}}\big)$ for each $T > 0$):

Theorem 2.5 (Reversibility in the gradient case)**.** *Let $\boldsymbol{\theta}$ denote a fixed $d \times d$ invertible matrix and let $\mathcal{F}$ be a set of compatible constraints. If Φ is a $\mathcal{C}^2$-function on $\mathbb{R}^d$ with bounded derivatives, then the solution of*

$$\mathbf{X}(t) = \mathbf{X}(0) + \boldsymbol{\theta}\mathbf{W}(t) - \frac{1}{2}\int_0^t \boldsymbol{\theta}\ {}^t\boldsymbol{\theta}\nabla\Phi(\mathbf{X}(s))ds + \sum_{f\in\mathcal{F}}\int_0^t \boldsymbol{\theta}\ {}^t\boldsymbol{\theta}\nabla f(\mathbf{X}(t))d\mathbf{L}_f(s) \tag{2.2}$$

admits $d\mu(\mathbf{x}) = \mathbb{1}_{\mathcal{D}}(\mathbf{x})e^{-\Phi(\mathbf{x})}d\mathbf{x}$ as a time-reversible measure.

The existence and reversibility of a weak solution of (2.2) is a simple special case of [3] if the domain $\mathcal{D}$ is bounded: the constraints are smooth enough for a regular exhaustion of $\mathcal{D}$ to admit a uniform bound on the surface measures of the boundaries. Thus $\mathcal{D}$ complies with the assumptions of theorem 5.1 in [3]. However the small illustration in section 3 and some realistic applications as in [9] involve unbounded domains.

The remaining of this section is devoted to the proofs of the above results. We first prove lemmas 2.3 and 2.4 which will be useful in the other proofs and then proceed to theorems 2.2 and 2.5.

Proof of lemma 2.3. The third compatibility condition is

$$\exists \beta_0 > 0\ \ \forall \mathbf{x} \in \partial\mathcal{D}\ \ \delta(0, \mathrm{Conv}(\mathbf{x})) \geq \beta_0.$$

The condition in lemma 2.3 can be rewritten as

$$\exists \beta_0 > 0\ \forall \mathbf{x} \in \partial\mathcal{D} \quad \max_{\mathbf{v}\neq 0} \min \left\{ \frac{\mathbf{v}}{|\mathbf{v}|}.\frac{\nabla f(\mathbf{x})}{|\nabla f(\mathbf{x})|};\ f \in \mathcal{F},\ f(\mathbf{x}) = 0 \right\} \geq \beta_0.$$

Thus it suffices to prove that for each $\mathbf{x} \in \partial\mathcal{D}$

$$\delta(0, \mathrm{Conv}(\mathbf{x})) = \max_{|\mathbf{v}|=1} \min \left\{ \mathbf{v}.\frac{\nabla f(\mathbf{x})}{|\nabla f(\mathbf{x})|};\ f \in \mathcal{F},\ f(\mathbf{x}) = 0 \right\}.$$

The lower bound on $\delta(0, \mathrm{Conv}(\mathbf{x}))$ follows from the inequality

$$|\mathbf{y}| \geq \mathbf{y}.\mathbf{v} \geq \min_{f\in\mathcal{F}, f(\mathbf{x})=0} \frac{\nabla f(\mathbf{x})}{|\nabla f(\mathbf{x})|}.\mathbf{v}$$

which holds for every unit vector $\mathbf{v}$ and every $\mathbf{y} \in \mathrm{Conv}(\mathbf{x})$ because families (c_f) of non-negative numbers summing up to 1 satisfy

$$\left(\sum_{f, f(\mathbf{x})=0} c_f \frac{\nabla f(\mathbf{x})}{|\nabla f(\mathbf{x})|} \right).\mathbf{v} \geq \left(\sum_{f, f(\mathbf{x})=0} c_f \right) \min_{f, f(\mathbf{x})=0} \frac{\nabla f(\mathbf{x})}{|\nabla f(\mathbf{x})|}.\mathbf{v}$$

Since the convex hull $\mathrm{Conv}(\mathbf{x})$ is a closed set, it contains an element $\mathbf{z}$ with minimal norm: $|\mathbf{z}| = \delta(0, \mathrm{Conv}(\mathbf{x}))$. For each f satisfying $f(\mathbf{x}) = 0$ and for each positive ε, the convex combination $\frac{1}{1+\varepsilon}\left(\mathbf{z} + \varepsilon\, \frac{\nabla f(\mathbf{x})}{|\nabla f(\mathbf{x})|}\right)$ belongs to the convex hull hence its norm can not be smaller than $|\mathbf{z}|$:

$$|\mathbf{z}|^2 + \varepsilon^2 + 2\,\varepsilon\,\mathbf{z}.\frac{\nabla f(\mathbf{x})}{|\nabla f(\mathbf{x})|} \geq (1+\varepsilon)^2\,|\mathbf{z}|^2 \qquad \text{i.e.} \qquad \varepsilon + 2\,\mathbf{z}.\frac{\nabla f(\mathbf{x})}{|\nabla f(\mathbf{x})|} \geq (2+\varepsilon)|\mathbf{z}|^2$$

This proves that $\dfrac{\mathbf{z}}{|\mathbf{z}|}.\dfrac{\nabla f(\mathbf{x})}{|\nabla f(\mathbf{x})|} \geq |\mathbf{z}| = \delta(0, \mathrm{Conv}(\mathbf{x}))$ and provides the upper bound on $\delta(0, \mathrm{Conv}(\mathbf{x}))$. □

Proof of lemma 2.4. Let us prove the compatibility of the set $\mathcal{F}^{\boldsymbol{\theta}} = \{g(\cdot) = f(\boldsymbol{\theta}\,\cdot);\ f \in \mathcal{F}\}$ of transformed constraints. $\boldsymbol{\theta}^{-1}\mathcal{D} = \left\{\mathbf{y} \in \mathbb{R}^d;\ \forall f \in \mathcal{F}\ f(\boldsymbol{\theta}\mathbf{y}) > 0\right\}$ is a non-empty connected set as continuous image of the non-empty connected set $\mathcal{D}$. $\boldsymbol{\theta}$ also transforms the bounds on the f's into bounds on the g's. Lemma 2.3 with $\mathbf{v}$ replaced by $\boldsymbol{\theta}\mathbf{v}$ provides the existence of some positive β_0 such that

$$\forall \mathbf{x} \in \partial\mathcal{D} \quad \exists \mathbf{v} \neq 0 \quad \forall f \in \mathcal{F} \text{ s.t. } f(\mathbf{x}) = 0 \quad \mathbf{v}.{}^t\boldsymbol{\theta}\nabla f(\mathbf{x}) \geq \beta_0 |\boldsymbol{\theta}\mathbf{v}|\, |\nabla f(\mathbf{x})|.$$

Replacing $\mathbf{x}$ by $\boldsymbol{\theta}\mathbf{y}$ we obtain

$$\forall \mathbf{y} \in \partial(\boldsymbol{\theta}^{-1}\mathcal{D}) \quad \exists \mathbf{v} \neq 0 \quad \forall g \in \mathcal{F}^{\boldsymbol{\theta}} \text{ s.t. } g(\mathbf{y}) = 0$$

$$\mathbf{v}.\nabla g(\mathbf{y}) \geq \beta_0 |\boldsymbol{\theta}\mathbf{v}|\, |{}^t\boldsymbol{\theta}^{-1}\nabla g(\mathbf{y})| \geq \beta_0 \frac{|\mathbf{v}|}{|\boldsymbol{\theta}^{-1}|} \frac{|\nabla g(\mathbf{y})|}{|{}^t\boldsymbol{\theta}|}.$$

Thanks to lemma 2.3 with $\beta_0' = \frac{\beta_0}{|\boldsymbol{\theta}^{-1}|\,|{}^t\boldsymbol{\theta}|}$, this proves that $\mathcal{F}^{\boldsymbol{\theta}}$ is a set of compatible constraints.

In order to prove the second part of lemma 2.4, we now assume that $f(\underline{\mathbf{x}}, x_d) = f(\underline{\mathbf{x}}, 0)$ for each f in $\mathcal{F}$ and each $(\underline{\mathbf{x}}, x_d)$ in $\mathbb{R}^d$. The set $\mathcal{D} = \{\mathbf{x} \in \mathbb{R}^d;\ f(\mathbf{x}) > 0\}$ is equal to $\underline{\mathcal{D}} \times \mathbb{R}$ where $\underline{\mathcal{D}} = \{\mathbf{z} \in \mathbb{R}^{d-1};\ \underline{f}(\mathbf{z}) > 0\}$ is a non empty connected set as a projection of a non-empty connected set. The lower bound on ∇f and the upper bound on $D^2 f$ transfer to $\underline{f}$ because $\nabla f = (\nabla \underline{f}, 0)$ and $|D^2 f(\mathbf{x})| = |D^2 f(x_1, \cdots, x_{d-1}, 0)|$. From the compatibility of $\mathcal{F}$, we also get the existence of a positive β_0 such that for each $\mathbf{x} \in \partial\mathcal{D}$ there exists a unit vector $\mathbf{v}$ satisfying $\mathbf{v}.\nabla f(\mathbf{x}) \geq \beta_0 |\nabla f(\mathbf{x})|$ for each function $f \in \mathcal{F}$ vanishing at point $\mathbf{x}$. The last coordinate of $\nabla f(\mathbf{x})$ vanishes hence $\underline{\mathbf{v}} = (v_1, \cdots, v_{d-1}) \neq 0$. Since $\partial\mathcal{D} = \partial\underline{\mathcal{D}} \times \mathbb{R}$ we obtain the compatibility of the $\underline{f}$'s:

$$\exists \beta_0 > 0 \quad \forall \mathbf{z} \in \partial\underline{\mathcal{D}} \quad \exists \underline{\mathbf{v}} \neq 0 \quad \forall f \in \mathcal{F} \text{ s.t. } \underline{f}(\mathbf{z}) = 0 \quad \underline{\mathbf{v}}.\nabla \underline{f}(\mathbf{z}) \geq \beta_0 |\underline{\mathbf{v}}|\, |\nabla \underline{f}(\mathbf{z})|$$

□

Proof of theorems 2.2 and 2.5.
The case of normal reflection: we assume here that $\boldsymbol{\theta} = I_d$. According to corollary 3.6 of [5], equation (2.1) has a unique strong solution as soon as $\mathcal{D}$ satisfies the four assumptions of the inheritance criterion for Uniform Exterior Sphere and Uniform Normal Cone conditions (proposition 3.4 in [5]). We will check these four assumptions in the unusual order (i) (ii) (iv) (iii) because some parameter appearing in (iii) depends on a parameter defined in (iv). We use the notations $\underline{\nabla f} := \inf\{|\nabla f|(\mathbf{x});\ \mathbf{x} \in \overline{\mathcal{D}},\ f(\mathbf{x}) = 0\}$ and $||D^2 f||_\infty := \sup\{|D^2 f|(\mathbf{x});\ \mathbf{x} \in \mathbb{R}^d\}$.

Assumption (i): We have to prove that $\left\{\mathbf{x} \in \mathbb{R}^d\ ;\ f(\mathbf{x}) \geq 0\right\}$ has $\mathcal{C}^2$ boundary in $\overline{\mathcal{D}}$ for each constraint f. Let us fix $\mathbf{x} \in \overline{\mathcal{D}}$ such that $f(\mathbf{x}) = 0$. By definition of the constraint functions $\nabla f(\mathbf{x}) \neq 0$, that is, we can choose an index k such that $\nabla_k f(\mathbf{x}) \neq 0$. For simplicity sake we assume that $\nabla_d f(\mathbf{x}) > 0$ (the idea easily adapts to $k \neq d$ and to negative partial derivatives). Applying the implicit function theorem to the $\mathcal{C}^2$-function f, we obtain the existence of a neighborhood V of $(x_1, \dots, x_{d-1})$, a neighborhood U' of x_d and an increasing $\mathcal{C}^2$-function h such that the $\mathcal{C}^2$-diffeomorphism $(y_1, \dots, y_d) \longmapsto (y_1, \dots, y_{d-1}, f(y_1, \dots, y_d))$ maps $\{\mathbf{y} \in V \times U';\ f(\mathbf{y}) \geq 0\}$ to

$$\{(y_1, \dots, y_{d-1}, z_d) \in V \times U';\ z_d \geq h(y_1, \dots, y_{d-1}, 0)\}.$$

Hence the subset $\left\{\mathbf{x} \in \mathbb{R}^d;\ f(\mathbf{x}) \geq 0\right\}$ has $\mathcal{C}^2$ boundary in $\overline{\mathcal{D}}$ and its inward normal direction at point $\mathbf{x}$ is $\dfrac{\nabla f(\mathbf{x})}{|\nabla f(\mathbf{x})|}$.

Assumption (ii): Let us prove that $\left\{\mathbf{x} \in \mathbb{R}^d;\ f(\mathbf{x}) \geq 0\right\}$ satisfies the Uniform Exterior Sphere property restricted to $\overline{\mathcal{D}}$. According to definition 3.1 in [5], we have to prove that there exists some positive α_f such that, for each $\mathbf{x} \in \overline{\mathcal{D}}$ satisfying $f(\mathbf{x}) = 0$, one has

$$\forall \mathbf{y} \text{ s.t. } f(\mathbf{y}) \geq 0 \qquad (\mathbf{y} - \mathbf{x}).\frac{\nabla f(\mathbf{x})}{|\nabla f(\mathbf{x})|} + \frac{1}{2\alpha_f}|\mathbf{y} - \mathbf{x}|^2 \geq 0. \tag{2.3}$$

Let us fix $\mathbf{x} \in \overline{\mathcal{D}}$ on which f vanish. Taylor formula gives

$$\nabla f(\mathbf{x}).(\mathbf{y} - \mathbf{x}) + \frac{1}{2}(\mathbf{y} - \mathbf{x}).D^2 f(\mathbf{x} + c^*(\mathbf{y} - \mathbf{x}))(\mathbf{y} - \mathbf{x}) = f(\mathbf{y})$$

for each $\mathbf{y} \in \mathbb{R}^d$ with some $c^* \in [0;1]$ depending on $\mathbf{y}$ and $\mathbf{x}$. In particular, for $\mathbf{y}$ such that $f(\mathbf{y}) \geq 0$ we obtain $(\mathbf{y} - \mathbf{x}).\dfrac{\nabla f(\mathbf{x})}{|\nabla f(\mathbf{x})|} + \dfrac{||D^2 f||_\infty}{2|\nabla f(\mathbf{x})|}|\mathbf{y} - \mathbf{x}|^2 \geq 0$ which gives (2.3) with $\alpha_f = \dfrac{\underline{\nabla f}}{||D^2 f||_\infty}$.

Assumption (iv): We have to prove the existence of some $\beta_0 > 0$ such that for each $\mathbf{x} \in \partial\mathcal{D}$ there exists a unit vector $\mathbf{l}^0_{\mathbf{x}}$ satisfying $\mathbf{l}^0_{\mathbf{x}}.\nabla f(\mathbf{x}) \geq \beta_0 |\nabla f|$ for each constraint such that $f(\mathbf{x}) = 0$. But this has already been done in lemma 2.3 with $\beta_0 = \inf_{\mathbf{x} \in \partial\mathcal{D}} d(0, \mathrm{Conv}(\mathbf{x}))$ and $\mathbf{l}^0_{\mathbf{x}} = \frac{\mathbf{z}}{|\mathbf{z}|}$ for some $\mathbf{z}$ with minimal norm in $\mathrm{Conv}(\mathbf{x})$.

Assumption (iii): We have to prove that each set $\left\{\mathbf{x} \in \mathbb{R}^d;\ f(\mathbf{x}) \geq 0\right\}$ satisfies the Uniform Normal Cone property restricted to $\overline{\mathcal{D}}$ with constant β_f smaller than $\beta_0^2/2$. Taylor formula for the derivative of f yields $\nabla f(\mathbf{y}) = \nabla f(\mathbf{x}) + D^2 f(\mathbf{x} + c^*(\mathbf{y} - \mathbf{x}))(\mathbf{y} - \mathbf{x})$ for some $c^* \in [0;1]$ depending on $\mathbf{y}$ and $\mathbf{x}$. We obtain for $\mathbf{x}$ and $\mathbf{y}$ on which f vanish

$$\frac{\nabla f(\mathbf{x}).\nabla f(\mathbf{y})}{|\nabla f(\mathbf{x})||\nabla f(\mathbf{y})|} = \frac{|\nabla f(\mathbf{x})|}{|\nabla f(\mathbf{y})|} + \frac{\nabla f(\mathbf{x}).D^2 f(\mathbf{x} + c^*(\mathbf{y} - \mathbf{x}))(\mathbf{y} - \mathbf{x})}{|\nabla f(\mathbf{x})||\nabla f(\mathbf{y})|}.$$

Since $|\nabla f(\mathbf{x})| \geq |\nabla f(\mathbf{y})| - |D^2 f(\mathbf{x} + c^*(\mathbf{y} - \mathbf{x}))(\mathbf{y} - \mathbf{x})|$ the right hand side is not smaller than

$$1 - \frac{|D^2 f(\mathbf{x} + c^*(\mathbf{y} - \mathbf{x}))(\mathbf{y} - \mathbf{x})|}{|\nabla f(\mathbf{y})|} - \frac{|\nabla f(\mathbf{x})||D^2 f(\mathbf{x} + c^*(\mathbf{y} - \mathbf{x}))(\mathbf{y} - \mathbf{x})|}{|\nabla f(\mathbf{x})||\nabla f(\mathbf{y})|}$$

i.e. $\dfrac{\nabla f(\mathbf{x})}{|\nabla f(\mathbf{x})|}.\dfrac{\nabla f(\mathbf{y})}{|\nabla f(\mathbf{y})|} \geq 1 - 2\dfrac{||D^2 f||_\infty}{\underline{\nabla f}}|\mathbf{y} - \mathbf{x}|$. As a consequence, for any $\beta_f \in]0,1[$ one can choose a $\delta_f > 0$ small enough such that for each $\mathbf{x} \in \overline{\mathcal{D}}$ satisfying $f(\mathbf{x}) = 0$ and each $\mathbf{y} \in \overline{\mathcal{D}}$ satisfying $f(\mathbf{y}) = 0$ and $|\mathbf{y} - \mathbf{x}| \leq \delta_f$ one has $\dfrac{\nabla f(\mathbf{y})}{|\nabla f(\mathbf{y})|}.\dfrac{\nabla f(\mathbf{x})}{|\nabla f(\mathbf{x})|} \geq \sqrt{1 - \beta_f^2}$.

This proves that $\left\{\mathbf{x} \in \mathbb{R}^d;\ f(\mathbf{x}) \geq 0\right\}$ satisfies the Uniform Normal Cone property restricted to $\overline{\mathcal{D}}$ with any constant $\beta_f \in]0;1[$. In particular it is satisfied with $\beta_f < \beta_0^2/2$ as requested.

To complete the proof of theorems 2.2 and 2.5 for $\boldsymbol{\theta} = I_d$, we proceed as in the proof of theorem 3.3 in [5], replacing the probability measure $d\mu(\mathbf{x}) = \frac{1}{Z}\mathbb{1}_{\mathcal{D}}(\mathbf{x})e^{-\Phi(\mathbf{x})}d\mathbf{x}$

in that proof by the (σ-finite but maybe unbounded) measure μ defined by $d\mu(\mathbf{x}) = \mathbb{1}_{\mathcal{D}}(\mathbf{x})e^{-\Phi(\mathbf{x})}d\mathbf{x}$. Girsanov theorem yields the density of the distribution of the process with initial measure μ with respect to the distribution of reflected Brownian motion with Lebesgue measure as initial measure. Since both this density and the distribution of reflected Brownian motion starting from Lebesgue measure are time-reversal invariant, we obtain the reversibility of the solution with initial measure μ.

The case of co-normal reflection: Let us check that the results obtained in the normal reflection case $\boldsymbol{\theta} = I_d$ transfer to the case of any invertible matrix $\boldsymbol{\theta}$. Using the notation $\mathbf{X}^{\boldsymbol{\theta}} = \boldsymbol{\theta}^{-1}\mathbf{X}$, existence and uniqueness for equation (2.1) is equivalent to existence and uniqueness for

$$\mathbf{X}^{\boldsymbol{\theta}}(t) = \mathbf{X}^{\boldsymbol{\theta}}(0)+\int_0^t \boldsymbol{\theta}^{-1}\boldsymbol{\sigma}(\boldsymbol{\theta}\mathbf{X}^{\boldsymbol{\theta}}(s))d\mathbf{W}(s)+\int_0^t \boldsymbol{\theta}^{-1}\mathbf{b}(\boldsymbol{\theta}\mathbf{X}^{\boldsymbol{\theta}}(s))ds+\sum_{f\in\mathcal{F}}\int_0^t {}^t\boldsymbol{\theta}\nabla f(\boldsymbol{\theta}\mathbf{X}^{\boldsymbol{\theta}}(s))dL_f(s) \tag{2.4}$$

in the closure of the set $\boldsymbol{\theta}^{-1}\mathcal{D} = \left\{\mathbf{y}\in\mathbb{R}^d;\ \forall f\in\mathcal{F}\ f(\boldsymbol{\theta}\mathbf{y})>0\right\}$ with local times satisfying the condition $L_f(\cdot) = \int_0^{\cdot} \mathbb{1}_{f(\boldsymbol{\theta}\mathbf{X}^{\boldsymbol{\theta}}(s))=0}\ dL_f(s)$.

The transformed coefficients $\boldsymbol{\sigma}^{\boldsymbol{\theta}} = \boldsymbol{\theta}^{-1}\boldsymbol{\sigma}(\boldsymbol{\theta}\ \cdot)$ and $\mathbf{b}^{\boldsymbol{\theta}} = \boldsymbol{\theta}^{-1}\mathbf{b}(\boldsymbol{\theta}\ \cdot)$ inherit the boundedness and Lipschitz continuity property from $\boldsymbol{\sigma}$ and $\mathbf{b}$. Lemma 2.4 provides the compatibility of the set of transformed constraints $\{f(\boldsymbol{\theta}\ \cdot);\ f\in\mathcal{F}\}$. Moreover, (2.4) is an equation with normal reflection because $\nabla(f(\boldsymbol{\theta}\ \cdot)) = {}^t\boldsymbol{\theta}\nabla f(\boldsymbol{\theta}\ \cdot)$. Thus equation (2.4) and then equation (2.1) have a unique strong solution.

Moreover, if $\boldsymbol{\sigma} = \boldsymbol{\theta}$, $\mathbf{b} = -\frac{1}{2}\boldsymbol{\theta}{}^t\boldsymbol{\theta}\nabla\Phi$ and $\mathbf{X}(0) \sim \mathbb{1}_{\mathcal{D}}(\mathbf{x})e^{-\Phi(\mathbf{x})}d\mathbf{x}$ for some $\mathcal{C}^2$-function Φ with bounded derivatives, then $\mathbf{X}^{\boldsymbol{\theta}}$ is the solution of equation (2.4) with $\boldsymbol{\sigma}^{\boldsymbol{\theta}} = I_d$, $\mathbf{b}^{\boldsymbol{\theta}} = -\frac{1}{2}{}^t\boldsymbol{\theta}\nabla\Phi(\boldsymbol{\theta}\ \cdot)$ and initial distribution $\mathbf{X}^{\boldsymbol{\theta}}(0) \sim \mathbb{1}_{\boldsymbol{\theta}^{-1}\mathcal{D}}(\mathbf{y})e^{-\Phi(\boldsymbol{\theta}\mathbf{y})}|det(\boldsymbol{\theta})|d\mathbf{y}$. Thanks to the reversibility result obtained for normal reflection, $\mathbf{X}^{\boldsymbol{\theta}}$ is time-reversible. This implies the time-reversibility of the solution of equation (2.1). □

3 Example: cluster of particles around an attractive sphere

Our aim in theorem 2.2 is to easily obtain the existence of dynamics derived from physical models, so that we can concentrate on their ergodicity properties. We are interested in the convergence toward equilibrium for colloidal particles as in [9]. However, the study of the Janus particles described in [9] is complicated by the fact that these spherical particles have an additional characteristic beside their position, which is an angular characterictic. In this note, we restrict ourselves to a small illustration of the previous results and we consider particles which have a simpler additional characteristic: a random radius.

We study the configuration of a large number of such particles around a fixed sphere we call the planet. These spherical hard particles have a random radius oscillating between a minimum and a maximum value (as in [5]). Each particle is driven by a Brownian motion and undergoes the influence of the gravitational attraction generated by the planet. The motion is perturbated as the particles bump into each other and into the planet. In this illustration we obtain the existence and uniqueness of such a dynamics and we describe typical configurations of the equilibrium distribution of the particles. Using the results of section 2, we prove in proposition 3.3 that the particles eventually tend to cluster at the surface of the planet when the temperature (represented by the diffusion coefficient) tends to zero.

More precisely, the planet is the closed ball $B(0,R)$ in $\mathbb{R}^d$ centered at the origin with radius R. A large number n of particles moves around it. Each particle is represented by the position x_i of its center in $\mathbb{R}^d$ and the value $\breve{x}_i$ of its radius. Thus configurations are vectors $\mathbf{x} = (x_1, \breve{x}_1, \dots, x_n, \breve{x}_n)$ in $\mathbb{R}^{n(d+1)}$.

To prevent negative radii, we enforce $\breve{x}_i \in [r_-, r_+]$ for some fixed values $0 < r_- < r_+$.

Random oscillations of the positions of the particles are not on the same scale as random oscillations of their radii. The elasticity coefficient $\breve{\sigma} > 0$ of their surface takes this into account.

We assume that the gravity field φ generated by the planet is isotropic: it only depends on the norm $|x|$. As usual (see e.g. [2]) the gravitational attraction appears as a drift in the dynamics. Function φ is an increasing function which is $\mathcal{C}^2$ on $]0; +\infty[$. The drift decreases with the distance, but not too fast in the sense that $\varphi'' \leq 0$ and $\liminf_{\rho\to+\infty} \rho\varphi'(\rho) > 0$. An important example in dimension $d = 3$ is $\varphi(\rho) = C^{st}\ln(\rho)$ which gives the drift $-\varphi'(\rho) = -\frac{C^{st}}{\rho}$ corresponding to the gravitational acceleration $-\varphi''(\rho) = \frac{C^{st}}{\rho^2}$.

At temperature $\theta > 0$, the random motion of particles is modelized by the stochastic differential system

$$(\mathcal{E}_\theta)\begin{cases} \text{for } i \in \{1,\dots,n\} \\ X_i(t) = X_i(0) + \theta W_i(t) - \displaystyle\int_0^t \varphi'(|X_i(s)|)\frac{X_i}{|X_i|}(s)\,ds \\ \qquad\qquad + \displaystyle\int_0^t \frac{X_i}{R+\breve{X}_i}(s)\,dL_i^R(s) + \sum_{j=1}^n \int_0^t \frac{X_i - X_j}{\breve{X}_i + \breve{X}_j}(s)\,dL_{ij}(s) \\ \breve{X}_i(t) = \breve{X}_i(0) + \theta\breve{\sigma}\breve{W}_i(t) - \breve{\sigma}^2 L_i^R(t) - L_i^+(t) + L_i^-(t) - \breve{\sigma}^2 \displaystyle\sum_{j=1}^n L_{ij}(t) \end{cases}$$

In this equation, vector $(X_i(\cdot), \breve{X}_i(\cdot))_{1\leq i\leq n}$ represents the positions and radii of the n particles, the W_i's are independent $\mathbb{R}^d$-valued Brownian motions and the $\breve{W}_i$'s are independent one-dimensional Brownian motions, also independent from the W_i's. The amplitude of the Brownian oscillation of the position depends on temperature θ, while the amplitude of the radius oscillation depends on both the temperature θ and the surface elasticity $\breve{\sigma}$. The drift of X_i is directed toward the origin as expected. The local time L_i^R represents the repulsion received by the i^{th} particle when it collides with the planet (impulsion away from the origin in the direction of the unit vector $\frac{X_i}{R+\breve{X}_i}$) and the local times L_{ij} represent the collisions between particles, which tend to move the involved particles away from each other (unit direction $\frac{X_i - X_j}{\breve{X}_i+\breve{X}_j}$). Collisions between particles are symmetric ($L_{ij} \equiv L_{ji}$). These local times also appear in the dynamics of the radii, because particles, like bubbles, have smaller radii after the collision. The local times L_i^+ and L_i^- are here to comply with the condition $\breve{x}_i \in [r_-, r_+]$ and give a positive (resp. negative) impulsion to the radius if it becomes too small (resp. too large). The impulsions are only given on the boundary of the set of allowed configurations, therefore L_i^R's, L_i^+'s, L_i^-'s and L_{ij}'s should satisfy

$$(\mathcal{E}'_\theta)\begin{cases} \text{for } i,j \in \{1,\dots,n\} \\ L_i^R(t) = \displaystyle\int_0^t \mathbb{1}_{|X_i(s)|=R+\breve{X}_i(s)}\,dL_i^R(s)\ , \quad L_i^+(t) = \int_0^t \mathbb{1}_{\breve{X}_i(s)=r_+}\,dL_i^+(s) \\ L_i^-(t) = \displaystyle\int_0^t \mathbb{1}_{\breve{X}_i(s)=r_-}\,dL_i^-(s)\ , \quad L_{ij}(t) = \int_0^t \mathbb{1}_{|X_i(s)-X_j(s)|=\breve{X}_i(s)+\breve{X}_j(s)}\,dL_{ij}(s) \end{cases}$$

The corresponding set of constraints is

- $f_i^R(\mathbf{x}) = |x_i|^2 - (R+\breve{x}_i)^2 > 0$ for $1 \leq i \leq n$ (particles do not intersect the planet);
- $f_i^+(\mathbf{x}) = r_+ - \breve{x}_i > 0$ for $1 \leq i \leq n$ (radii are smaller than the maximum value);
- $f_i^-(\mathbf{x}) = \breve{x}_i - r_- > 0$ for $1 \leq i \leq n$ (radii are larger than the minimum value);
- $f_{ij}(\mathbf{x}) = |x_i - x_j|^2 - (\breve{x}_i + \breve{x}_j)^2 > 0$ for $i \neq j$ in $\{1, 2, \dots, n\}$ (particles do not overlap).

Proposition 3.1.
$\left\{f_i^R, f_i^+, f_i^- ;\ 1 \le i \le n\right\} \cup \{f_{ij};\ 1 \le i < j \le n\}$ is a set of compatible constraints on $\mathbb{R}^{n(d+1)}$.

Let $\mathcal{D} = \bigcap_{i=1}^n \left((f_i^R)^{-1}(\mathbb{R}_+^*) \cap (f_i^+)^{-1}(\mathbb{R}_+^*) \cap (f_i^+)^{-1}(\mathbb{R}_+^*) \cap \bigcap_{j\neq i} (f_{ij})^{-1}(\mathbb{R}_+^*) \right)$.

Proposition 3.2.
If φ is an increasing $\mathcal{C}^2$-function on $]0;+\infty[$ satisfying $\varphi'' \le 0$ and $\liminf_{\rho\to+\infty} \rho\varphi'(\rho) > 0$ then equation $(\mathcal{E}_\theta, \mathcal{E}'_\theta)$ has a unique strong solution, which is a $\overline{\mathcal{D}}$-valued process.
The measure $\mathbb{1}_{\mathcal{D}}(\mathbf{x}) e^{-\frac{1}{\theta^2}\sum_{i=1}^n \varphi(|x_i|)} d\mathbf{x}$ is a time-reversible measure for the solution. For θ small enough, this measure is finite thus the solution admits a time-reversible probability measure:

$$\mu_\theta(d\mathbf{x}) = \frac{1}{\int_{\mathcal{D}} e^{-\frac{1}{\theta^2}\sum_{i=1}^n \varphi(|y_i|)} d\mathbf{y}} \mathbb{1}_{\mathcal{D}}(\mathbf{x}) e^{-\frac{1}{\theta^2}\sum_{i=1}^n \varphi(|x_i|)} d\mathbf{x}$$

Once existence and uniqueness is proved for the dynamics, we will check that at low temperature all particles cluster around the planet with high probability. That is, there exists with high probability an interface between two regions around the planet: no particle over some altitude, and beneath this altitude a particle density so high that one cannot add one more particle (see figure 1).

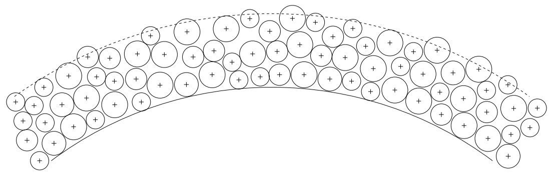

Figure 1: A configuration with an interface between high particle density and empty space.

Proposition 3.3.
For each positive ε, let A_ε be the set of configurations which do not pack into a minimal volume:

$$A_\varepsilon = \{\mathbf{x} \in \mathcal{D};\ \exists \mathbf{y} \in \mathcal{D}\ \exists k \le n \text{ s.t. } \forall i \neq k\ \ y_i = x_i \text{ and } |y_k| < |x_k| - \varepsilon\}$$

The probability that A_ε occurs at equilibrium tends to zero as the temperature tends to zero:

$$\lim_{\theta\to 0} \mu_\theta(A_\varepsilon) = 0.$$

The end of the paper is devoted to the proofs of the three above propositions.

Proof of proposition 3.1. The constraints in

$$\mathcal{F} = \{f_{ij}\ ;\ 1 \le i < j \le n\} \cup \left\{f_i^+, f_i^-, f_i^R\ ;\ 1 \le i \le n\right\}$$

are $\mathcal{C}^\infty$ and the corresponding set $\mathcal{D}$ of possible configurations is obviously a non-empty connected set. The first derivative of each constraint function is uniformly positive on its vanishing set because:

- $\nabla f_i^R(\mathbf{x}) = 2\,(0,\dots,0,x_i,-(R+\breve{x}_i),0,\dots,0)$
  if $f_i^R(\mathbf{x}) = 0$ i.e. $|x_i| = R + \breve{x}_i$ then $|\nabla f_i^R(\mathbf{x})| = 2\sqrt{2}(R+\breve{x}_i) \ge 2\sqrt{2}(R+r_-) > 0$;
- $\nabla f_i^+(\mathbf{x}) = -\nabla f_i^-(\mathbf{x}) = -\,(0,\dots,0,1,0,\dots,0)$ $\quad$ (($i(d+1)-1$)th coordinate) ;

- $\nabla f_{ij}(\mathbf{x}) = 2\,(0,\ldots,0,x_i-x_j,-(\breve{x}_i+\breve{x}_j),0,\ldots,0,x_j-x_i,-(\breve{x}_i+\breve{x}_j),0,\ldots,0)$
  if $f_{ij}(\mathbf{x})=0$ i.e. $|x_i-x_j|=\breve{x}_i+\breve{x}_j$ then $|\nabla f_{ij}(\mathbf{x})| = 4(\breve{x}_i+\breve{x}_j) \geq 8r_- > 0$.

We check the condition $\inf\limits_{\mathbf{x}\in\partial\mathcal{D}} d(0,\mathrm{Conv}(\mathbf{x}))>0$ in the form given in lemma 2.3. We have to find some positive β_0 and some non-vanishing vector $\mathbf{v}$ depending on $\mathbf{x}\in\partial\mathcal{D}$ such that

$$\forall f\in\mathcal{F} \text{ s.t. } f(\mathbf{x})=0 \quad \mathbf{v}.\nabla f(\mathbf{x}) \geq \beta_0|\mathbf{v}|\;|\nabla f(\mathbf{x})|$$

From an intuitive point of view, $\mathbf{v}$ is the "shortest way to go back" into $\mathcal{D}$ from the point $\mathbf{x}$ on the boundary of $\mathcal{D}$. It is the quickest way for colliding particles to go apart, for particles with maximum (resp. minimum) radius to become smaller (resp. larger) and for particles touching the planet to go away. C^R will denote the indices of these globules: $C^R=\{i \text{ s.t. } |x_i|=R+\breve{x}_i\}$.

Intuitively, the best way to separate colliding particles is to move them away from the center of gravity of the cluster. One should give each center x_i an impulsion in the direction $x_i - \frac{1}{\sharp C_i}\sum_{j\in C_i} x_j$ where $C_i\subset\{1,\ldots,n\}$ is the cluster of colliding particles around x_i (i.e. C_i is the set containing i and all indices connected to i in the graph constructed on the vertices $\{1,\ldots,n\}$ by the edges $j\sim j' \iff |x_j-x_{j'}|=\breve{x}_j+\breve{x}_{j'}$). Similarly, the best way for particles touching the planet to go away is for each center x_i with $i\in C^R$ to receive a small impulsion proportional to x_i (this impulsion will also separate clusters of colliding particles). So a convenient $\mathbf{v}$ should be

$$v_i = \begin{cases} x_i - \dfrac{1}{\sharp C_i}\displaystyle\sum_{j\in C_i} x_j & \text{if } C_i\cap C^R=\emptyset \\ x_i & \text{if } C_i\cap C^R\neq\emptyset \end{cases} \quad \text{and} \quad \breve{v}_i = \begin{cases} r_-/2 & \text{if } \breve{x}_i = r_- \\ -r_-/2 & \text{if } \breve{x}_i=r_+ \\ 0 \text{ otherwise} \end{cases}$$

Let us prove that the above vector $\mathbf{v}$ satisfies the desired inequalities.

- if $|x_i|=R+\breve{x}_i$ then $v_i=x_i$ hence $\quad \mathbf{v}.\dfrac{\nabla f_i^R(\mathbf{x})}{|\nabla f_i^R(\mathbf{x})|} = \dfrac{R+\breve{x}_i}{\sqrt{2}} - \dfrac{\breve{v}_i}{\sqrt{2}} \geq \dfrac{R}{\sqrt{2}}$
- if $\breve{x}_i=r_+$ then $\mathbf{v}.\dfrac{\nabla f_i^+(\mathbf{x})}{|\nabla f_i^+(\mathbf{x})|} = -\breve{v}_i = \dfrac{r_-}{2}$ and if $\breve{x}_i=r_-$ then $\mathbf{v}.\dfrac{\nabla f_i^-(\mathbf{x})}{|\nabla f_i^-(\mathbf{x})|} = \breve{v}_i = \dfrac{r_-}{2}$
- If $|x_i-x_j|=\breve{x}_i+\breve{x}_j$ then $C_i=C_j$ which implies $v_i-v_j=x_i-x_j$ thus

$$\mathbf{v}.\frac{\nabla f_{ij}(\mathbf{x})}{|\nabla f_{ij}(\mathbf{x})|} = \frac{\breve{x}_i+\breve{x}_j}{4} - \frac{\breve{v}_i+\breve{v}_j}{4} \geq \frac{r_-}{4}$$

So $\mathbf{v}.\frac{\nabla f(\mathbf{x})}{|\nabla f(\mathbf{x})|}$ is bounded from below, uniformly in $\mathbf{x}\in\partial\mathcal{D}$ and $f\in\mathcal{F}$ such that $f(\mathbf{x})=0$. To complete the proof of proposition 3.1, it only remains to find a uniform upper bound for $|\mathbf{v}|$.

$$|\mathbf{v}|^2 = \sum_{i=1}^n |v_i|^2+\breve{v}_i^2 = \sum_{i;\ C_i\cap C^R\neq\emptyset} |x_i|^2 + \sum_{i;\ C_i\cap C^R=\emptyset} |\frac{1}{\sharp C_i}\sum_{j\in C_i}(x_i-x_j)|^2 + n\frac{r_-^2}{4}$$

If C_i is any cluster of colliding globules,

$$\left|\sum_{j\in C_i}(x_i-x_j)\right|^2 \leq \sharp C_i\sum_{j\in C_i}|x_i-x_j|^2 \leq \sharp C_i\sum_{k=0}^{\sharp C_i-1}(2kr_+)^2 = (2r_+)^2(\sharp C_i)^2\frac{(\sharp C_i-1)(2\sharp C_i-1)}{6}$$

Similarly, if C_i is a cluster with at least one globule at distance $R+\breve{x}_i$ of the origin,

$$\sum_{j\in C_i}|x_j|^2 \leq \sum_{k=0}^{\sharp C_i-1}(R+\breve{x}_i+2kr_+)^2 \leq 2\sharp C_i(R+\breve{x}_i)^2 + 2(2r_+)^2\frac{(\sharp C_i-1)\sharp C_i(2\sharp C_i-1)}{6}$$

and the same upper bound holds for a sum over a union of such clusters. Consequently

$$|\mathbf{v}|^2 \le 2n(R+r_+)^2 + \frac{4}{3}r_+^2(n-1)n(2n-1) + \frac{2}{3}r_+^2 \sum_{i;\ C_i\cap C^R=\emptyset} (\sharp C_i - 1)(2\sharp C_i - 1) + n\frac{r_-^2}{4}$$

Since the sum over $\{i;\ C_i \cap C^R = \emptyset\}$ is smaller than $n(n-1)(2n-1)$, the norm of $\mathbf{v}$ is uniformly bounded from above as a function of $\mathbf{x}$. This completes the proof. □

Proof of proposition 3.2. We use theorem 2.2 with the $n(d+1)\times n(d+1)$ diagonal matrix $\boldsymbol{\theta}$ which has n times the sequence $(\theta,\dots,\theta,\theta\breve{\sigma})$ as its main diagonal entries. Since the constraints are compatible on $\mathbb{R}^{n(d+1)}$, for any $\mathcal{C}^2$-function Φ on $\mathbb{R}^{n(d+1)}$ with bounded derivatives,

$$\mathbf{X}(t) = \mathbf{X}(0) + \boldsymbol{\theta}\mathbf{W}(t) - \frac{1}{2}\int_0^t \boldsymbol{\theta}\,{}^t\boldsymbol{\theta}\nabla\Phi(\mathbf{X}(s))ds + \sum_{f\in\mathcal{F}}\int_0^t \boldsymbol{\theta}\,{}^t\boldsymbol{\theta}\nabla f(\mathbf{X}(s))dL_f(s) \qquad (3.1)$$

has a unique strong solution in the closure of the set $\mathcal{D}$ defined by the constraints. Choosing $\Phi(\mathbf{x}) = \sum_{i=1}^n \varphi(|x_i|)/\theta^2$ hence $\nabla_{x_i}\Phi(\mathbf{x}) = \frac{1}{\theta^2}\frac{x_i}{|x_i|}\varphi'(|x_i|)$ and $\nabla_{\breve{x}_i}\Phi(\mathbf{x}) = 0$, equation (3.1) becomes

$$\begin{cases} X_i(t) = X_i(0) + \theta W_i(t) - \displaystyle\int_0^t \varphi'(|X_i(s)|)\frac{X_i}{|X_i|}(s)ds + \int_0^t 2\theta^2 X_i(s)dL_{f_i^R}(s) \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad + \displaystyle\sum_{j=1}^n \int_0^t 2\theta^2(X_i - X_j)(s)dL_{f_{ij}}(s) \\ \breve{X}_i(t) = \breve{X}_i(0) + \theta\breve{\sigma}\breve{W}_i(t) + \theta^2\breve{\sigma}^2\Big(-\displaystyle\int_0^t 2(R+\breve{X}_i)(s)dL_{f_i^R}(s) - L_{f_i^+}(t) + L_{f_i^-}(t) \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad - \displaystyle\sum_{j=1}^n \int_0^t 2(\breve{X}_i + \breve{X}_j)(s)dL_{f_{ij}}(s)\Big) \end{cases}$$

Let us define $L_{ij}(\cdot) = 2\theta^2\int_0^\cdot(\breve{X}_i+\breve{X}_j)(s)dL_{f_{ij}}(s)$, $L_i^+ = \theta^2\breve{\sigma}^2 L_{f_i^+}$, $L_i^- = \theta^2\breve{\sigma}^2 L_{f_i^-}$ and $L_i^R(\cdot) = 2\theta^2\int_0^\cdot(R+\breve{X}_i)(s)dL_{f_i^R}(s)$. The property $L_f(\cdot) = \displaystyle\int_0^\cdot \mathbb{1}_{f(\mathbf{X}(s))=0}\, dL_f(s)$ implies that condition $(\mathcal{E}'_\theta)$ is satisfied for these new local times. Then the solution of equation (3.1) is the solution of $(\mathcal{E}_\theta)$. Theorem 2.5 states that $\mathbb{1}_{\mathcal{D}}(\mathbf{x})e^{-\Phi(\mathbf{x})}d\mathbf{x} = \mathbb{1}_{\mathcal{D}}(\mathbf{x})e^{-\frac{1}{\theta^2}\sum_{i=1}^n\varphi(|x_i|)}d\mathbf{x}$ is a time-reversible measure for the solution. To complete the proof, let us check that this measure can be renormalized as a probability measure for θ small enough.

From the positivity of $\ell := \liminf_{\rho\to+\infty}\rho\varphi'(\rho)$ we get

$$\forall\eta>0\ \ \exists K>0\ \ \forall\rho>K\ \ \varphi'(\rho) \ge \frac{\ell-\eta}{\rho}.$$

This integrates into $\varphi(\rho) \ge \varphi(K) + (\ell-\eta)(\ln\rho - \ln K)$ for $\rho \ge K$ and leads to

$$\forall c>0 \qquad \int_K^{+\infty} e^{-c\varphi(\rho)}\rho^{d-1}d\rho \le e^{-c\varphi(K)}K^{c(\ell-\eta)}\int_K^{+\infty}\rho^{-c(\ell-\eta)+d-1}d\rho$$

For c large enough to satisfy $-c(\ell-\eta)+d<0$ the above integral is finite, that is,

$$\int_{\mathbb{R}^d\setminus B(0,R)} e^{-c\varphi(|x|)}dx < +\infty$$

This gives the desired normalization constant for θ small enough to satisfy $\frac{1}{\theta^2} \ge c$:

$$\begin{aligned} \int_{\mathcal{D}} e^{-\frac{1}{\theta^2}\sum_{i=1}^n\varphi(|x_i|)}d\mathbf{x} &\le e^{-\frac{n}{\theta^2}\underline{\varphi}}\int_{(\mathbb{R}^d\setminus B(0,R))^n} e^{-c(\sum_{i=1}^n\varphi(|x_i|)-n\underline{\varphi})}d\mathbf{x} \\ &\le e^{cn\underline{\varphi}-\frac{n}{\theta^2}\underline{\varphi}}\left(\int_{\mathbb{R}^{d-1}\setminus B(0,R)} e^{-c\varphi(|x|)}dx\right)^n < +\infty \end{aligned}$$

where $\underline{\varphi} = \min_{[R;+\infty[} \varphi$ denotes the infimum on $[R;+\infty[$ of the smooth increasing function φ. ☐

Proof of proposition 3.3. Let $\underline{\varphi}_{\mathcal{D}} := \inf\{\sum_{i=1}^n \varphi(|y_i|);\ \mathbf{y} \in \mathcal{D}\}$. This infimum exists because φ is increasing on $]0;+\infty[$. We fix $\mathbf{x} \in A_\varepsilon$. There exists an allowed configuration $\mathbf{y}$ with all particles at the same position as in $\mathbf{x}$ except one particle (say, the k'th) which satisfies $|y_k| < |x_k| - \varepsilon$. Since φ' is a decreasing function,

$$\sum_{i=1}^n \varphi(|x_i|) = \sum_{i=1}^n \varphi(|y_i|) + \int_{|y_k|}^{|x_k|} \varphi'(\rho)d\rho > \underline{\varphi}_{\mathcal{D}} + (|x_k| - |y_k|)\varphi'(|x_k|)$$

Function φ' admits a limit at infinity.

- If this limit does not vanish, then $\sum_{i=1}^n \varphi(|x_i|) > \underline{\varphi}_{\mathcal{D}} + \varepsilon \lim_{\rho\to+\infty} \varphi'(\rho) > \underline{\varphi}_{\mathcal{D}}$;
- If $\lim_{+\infty} \varphi' = 0$, the positivity of $\ell = \liminf_{\rho\to+\infty} \rho\varphi'(\rho)$ implies the existence of a K such that

  $$\forall \rho \geq K \qquad \rho\varphi'(\rho) \geq \frac{2\ell}{3} \quad \text{and} \quad (R + r_+)\varphi'(\rho) \leq \frac{\ell}{3} \quad \text{hence} \quad (\rho - R - r_+)\varphi'(\rho) \geq \frac{\ell}{3}.$$

  Without loss of generality, we can choose $K \geq R + 2nr_+ + n\varepsilon$. Consider the x_k's such that there exists $\mathbf{y} \in \mathcal{D}$ satisfying $|y_k| < |x_k| - \varepsilon$ and $y_i = x_i$ for $i \neq k$.

  – If at least one of them has a norm smaller than K then

  $$\sum_{i=1}^n \varphi(|x_i|) > \underline{\varphi}_{\mathcal{D}} + \varepsilon\varphi'(K) > \underline{\varphi}_{\mathcal{D}}$$

  – If not, all particles in $\mathbf{x}$ are at distance at least K from the origin because it is impossible for only n particles to completely fill a sphere of radius $K \geq R+2nr_+ + n\varepsilon$. The x_k which has the largest norm is shifted at distance $R+r_+$ from the origin and is relabeled y_k. This define configuration $\mathbf{y} \in \mathcal{D}$. Then

  $$\sum_{i=1}^n \varphi(|x_i|) > \underline{\varphi}_{\mathcal{D}} + (|x_k| - R - r_+)\varphi'(|x_k|) \geq \underline{\varphi}_{\mathcal{D}} + \frac{\ell}{3} > \underline{\varphi}_{\mathcal{D}}$$

So we obtain $\sum_{i=1}^n \varphi(|x_i|) > \underline{\varphi}_{\mathcal{D}} + \varepsilon'$ for all $\mathbf{x} \in A_\varepsilon$ with a positive ε' equal to $\varepsilon \lim_{+\infty} \varphi'$ if this limit does not vanish and to $\min(\varepsilon\varphi'(K),\ \frac{\ell}{3})$ otherwise.

An immediate consequence is $\quad \mu_\theta(A_\varepsilon) \leq \mu_\theta(\{\mathbf{x} \in \mathcal{D};\ \sum_{i=1}^n \varphi(|x_i|) > \underline{\varphi}_{\mathcal{D}} + \varepsilon'\})$.

The normalization constant of the probability measure μ_θ is larger than

$$\int_{\mathcal{D}} \mathbb{1}_{\sum_{i=1}^n \varphi(|x_i|) \leq \underline{\varphi}_{\mathcal{D}} + \varepsilon'}\ e^{-\frac{1}{\theta^2}\sum_{i=1}^n \varphi(|x_i|)}\ d\mathbf{x} \geq e^{-\frac{1}{\theta^2}(\underline{\varphi}_{\mathcal{D}} + \varepsilon')} \int_{\mathcal{D}} \mathbb{1}_{\sum_{i=1}^n \varphi(|x_i|) \leq \underline{\varphi}_{\mathcal{D}} + \varepsilon'}\ d\mathbf{x}$$

thus $\quad \mu_\theta(A_\varepsilon) \leq \dfrac{\int_{\mathcal{D}} \mathbb{1}_{\sum_{i=1}^n \varphi(|x_i|) > \underline{\varphi}_{\mathcal{D}} + \varepsilon'}\ e^{-\frac{1}{\theta^2}(\sum_{i=1}^n \varphi(|x_i|) - \underline{\varphi}_{\mathcal{D}} - \varepsilon')}\ d\mathbf{x}}{\int_{\mathcal{D}} \mathbb{1}_{\sum_{i=1}^n \varphi(|x_i|) \leq \underline{\varphi}_{\mathcal{D}} + \varepsilon'}\ d\mathbf{x}}$.

The denominator does not depend on θ. Dominated convergence theorem ensures that the numerator converges to zero when θ tends to 0. So we obtain $\lim_{\theta\to 0} \mu_\theta(A_\varepsilon) = 0$. ☐

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