

**Weierstraß-Institut
für Angewandte Analysis und Stochastik
Leibniz-Institut im Forschungsverbund Berlin e. V.**

Preprint

ISSN 2198-5855

**Diffusion dynamics for an infinite system of two-type spheres and
the associated depletion effect**

Myriam Fradon¹, Julian Kern², Sylvie Roelly³, Alexander Zass²

submitted: June, 26

¹ Univ. Lille, CNRS UMR 8524
Laboratoire P. Painlevé
Bât. M2,
59655 Villeneuve d'Ascq Cedex,
France
E-Mail: myriam.fradon@univ-lille.fr

² Weierstrass Institute
Mohrenstr. 39
10117 Berlin
Germany
E-Mail: julian.kern@wias-berlin.de
alexander.zass@wias-berlin.de

³ University of Potsdam
Campus Golm, Haus 9
Karl-Liebknecht-Str. 24-25
D-14476 Potsdam OT Golm
Germany
E-mail: roelly@math.uni-potsdam.de

No. 3024
Berlin 2023



2020 *Mathematics Subject Classification.* 60K35; 60H10; 60J55; 82D99.

Key words and phrases. Stochastic differential equation, hard core interaction, reversible measure, collision local time, colloids, depletion interaction, Gibbs point process.

JK was partially funded by Deutsche Forschungsgemeinschaft (DFG) through grant CRC 1114 Scaling Cascades in Complex Systems, Project no. 235221301, Project C02 Interface dynamics: Bridging stochastic and hydrodynamic descriptions. AZ was funded by Deutsche Forschungsgemeinschaft (DFG) through DFG Project no. 422743078 The statistical mechanics of the interlacement point process in the context of SPP 2265 Random Geometric Systems. MF acknowledges support from the Labex CEMPI (ANR-11-LABX-0007-01).

Edited by
Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS)
Leibniz-Institut im Forschungsverbund Berlin e. V.
Mohrenstraße 39
10117 Berlin
Germany

Fax: +49 30 20372-303
E-Mail: preprint@wias-berlin.de
World Wide Web: <http://www.wias-berlin.de/>

Diffusion dynamics for an infinite system of two-type spheres and the associated depletion effect

Myriam Fradon, Julian Kern, Sylvie Rœlly, Alexander Zass

Abstract

We consider a random diffusion dynamics for an infinite system of hard spheres of two different sizes evolving in \mathbb{R}^d , its reversible probability measure, and its projection on the subset of the large spheres. The main feature is the occurrence of an attractive short-range dynamical interaction – known in the physics literature as a depletion interaction – between the large spheres, which is induced by the hidden presence of the small ones. By considering the asymptotic limit for such a system when the density of the particles is high, we also obtain a constructive dynamical approach to the famous discrete geometry problem of maximisation of the contact number of n identical spheres in \mathbb{R}^d . As support material, we propose numerical simulations in the form of movies.

1 Introduction: the model and its configuration space

Consider hard spheres randomly oscillating in a bath of very small free particles (see Figure 1) which are themselves independently randomly vibrating. At some appropriate scale, and as soon as two hard spheres are very close, one can observe the appearance of a strong mutual attraction which forces them to stay close together for a certain random amount of time. As no external force is acting on the system, this is a quite surprising phenomenon. What is going on?

To provide an answer, we provide here a mathematical formulation of this heuristics: in this introductory section, we first present the classical Asakura–Oosawa model from Chemical Physics, and then describe the mathematical setting of this work.

1.1 The origin of the model: a short heuristics

The model is the following: spheres of equal radius \hat{r} evolve in a bath of much smaller ones with radius $\hat{r} \ll \hat{r}$. The radius \hat{r} is called *depletion radius* for a reason which will become clear later. The larger spheres are *hard* in the sense that they cannot overlap: their interiors must always stay disjoint. The smaller spheres – called *particles* for clarity – which compose the (random) medium are also not allowed to overlap the large ones. This naturally leads to the presence of a virtual spherical shell around each large sphere, corresponding to the zone in which the centres of the particles are not allowed. This zone, called *depletion shell*, will play a fundamental role in what follows. Finally, the radius \hat{r} of the particles is taken so small that one can simplify the situation by considering them as an *ideal gas*: the particles can overlap each other. In Figure 1, a realisation of this model; the region coloured in orange is the union of the depletion shells.

This model is known in the physics literature as AO-model in reference to the seminal work of S. Asakura and F. Oosawa, who introduced in [1, 2] a size-asymmetric binary mixture in the Euclidean space \mathbb{R}^3 to describe colloids (large spheres) in a bath (or emulsion) of ideal polymers (the small particles) in the context of Chemical Physics, see also [25]. The reader can find in [18] a clear overview of the physical phenomenon and its modelling. Its importance is underlined by Binder, Virnau and Statt in [5]: “Since 60 years the Asakura–Oosawa model, which simply describes the polymers as ideal soft

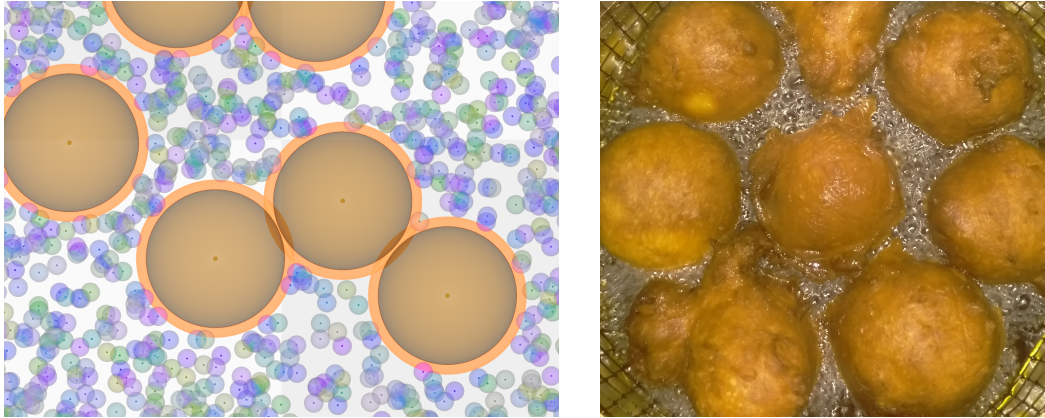


Figure 1: Identical hard spheres in a bath of identical small particles. An ideal mathematical representation (left) and a culinary realisation (right, jelly doughnuts in particles of frying oil).
Left: the orange depletion shells around the brown spheres overlap.

spheres, is an archetypal description for the statistical thermodynamics of such systems, accounting for many features of real colloid-polymer mixtures very well.” Indeed the bath of polymers induce a new attractive interaction between the colloids, called effective or *depletion interaction*. For a physical theoretical analysis of this general phenomena see, e.g., [19] and the valuable monograph [17]. As an illustration of the effect of the depletion force one can cite the ordered, helical conformation of long molecular chains like DNA in the Euclidean space \mathbb{R}^3 by interpreting this geometric structure as being thermodynamically induced by the entropy minimisation of depleting spheres, see [23].

A first rigorous mathematical treatment of the AO-model for an infinite number of both sphere types with methods of Statistical Mechanics appeared only recently in a series of papers by S. Jansen and coauthors, see [13, 14, 26].

1.2 The mathematical model

The geometric objects we deal with in this paper are spheres of two different types: the *hard spheres* with fixed radius \hat{r} and the *particles* with radius $\hat{r} < \hat{r}$. They are identified by the position of their centres in \mathbb{R}^d ; if a point $x \in \mathbb{R}^d$ is the centre of a hard sphere we denote it by \hat{x} , if it is the centre of a particle we denote it by \check{x} . In this way we can consider the set $\mathbb{X} = \hat{\mathbb{X}} \sqcup \check{\mathbb{X}} \simeq \mathbb{R}^d \times \{o, \cdot\}$ as duplication of \mathbb{R}^d , to distinguish between the two types of spheres.

Throughout the paper, the number of hard spheres will be finite and fixed, equal to $n \geq 1$.

The *configuration space* of the system is the set \mathcal{M} of σ -finite Radon point measures on \mathbb{X} , i.e., those of the form

$$\mathbf{x} = \hat{\mathbf{x}} + \check{\mathbf{x}} = \sum_{i=1}^n \delta_{\hat{x}_i} + \sum_{k \in K} \delta_{\check{x}_k}, \quad \hat{x}_i \in \hat{\mathbb{X}}, \check{x}_k \in \check{\mathbb{X}}, \quad K \subset \mathbb{N}^*,$$

such that for any compact $\Lambda \subset \mathbb{X}$, $\mathbf{x}(\Lambda) < +\infty$.

With this formalism, $\hat{\mathbf{x}}$ denotes the point measure of centres of hard spheres belonging to the configuration \mathbf{x} and $\check{\mathbf{x}}$ denotes the point measure of centres of the particles in \mathbf{x} . To simplify notations, we use interchangeably the notation \mathbf{x} for the point measure or for its support $\{\hat{x}_i, \check{x}_k, 1 \leq i \leq n, k \in K\} \subset \mathbb{R}^d$ (which is possible since the point measures we consider are a.s. simple), and write the

sum of two point measures as the juxtaposition $\overset{\circ}{\mathbf{x}}\dot{\mathbf{x}} := \overset{\circ}{\mathbf{x}} + \dot{\mathbf{x}}$. For $m \in \mathbb{N}$, let $\mathcal{M}_m \subset \mathcal{M}$ be the set of finite configurations with exactly m particles, that is

$$\mathcal{M}_m := \{\mathbf{x} = \overset{\circ}{\mathbf{x}}\dot{\mathbf{x}} \in \mathcal{M}, \dot{\mathbf{x}}(\dot{\mathbb{X}}) = m\}.$$

It is used in the first step of the proof of Theorem 2.1, to approximate the infinite configurations.

We write $\overset{\circ}{\mathcal{M}}$ (resp. $\dot{\mathcal{M}}$) for the point measures supported only by hard spheres (resp. particles).

In the following, $B(y, r)$ denotes the closed ball in \mathbb{R}^d centred in $y \in \mathbb{R}^d$ with radius $r \in \mathbb{R}_+$.

Under the non-overlap constraint, the configurations that can actually be realised, called *admissible*, make up the following subset $\mathcal{D} \subset \mathcal{M}$:

$$\mathcal{D} = \left\{ \overset{\circ}{\mathbf{x}} = \overset{\circ}{\mathbf{x}}\dot{\mathbf{x}} \in \mathcal{M} : \begin{array}{l} \forall i \neq j, \quad |\dot{x}_i - \dot{x}_j| \geq 2\dot{r}, \\ \forall i, k, \quad |\dot{x}_i - \dot{x}_k| \geq \dot{r} + \dot{r} \end{array} \right\}. \quad (1.1)$$

The second type of constraints in (1.1) can be interpreted as follows: around each hard sphere $B(\dot{x}_i, \dot{r})$ there is a shell of thickness \dot{r} , called *depletion shell*, that is forbidden for the centres of the particles $(\dot{x}_k)_k$, see Figure 1. We therefore introduce the radius $\overset{\circ}{\dot{r}}$, seen as an enlargement of the original hard-sphere radius \dot{r} :

$$\overset{\circ}{\dot{r}} := \dot{r} + \dot{r} = \dot{r}(1 + \rho), \quad \text{where } \rho := \frac{\dot{r}}{\dot{r}} \in [0, 1[, \quad (1.2)$$

and identify the forbidden area for particles around the admissible configuration of hard spheres $\overset{\circ}{\mathbf{x}}$ as the interior of

$$\mathbb{B}(\overset{\circ}{\mathbf{x}}) := \bigcup_{i=1}^n B(\dot{x}_i, \overset{\circ}{\dot{r}}) \subset \mathbb{R}^d. \quad (1.3)$$

As we will see in the paper, the parameter ρ defined in (1.2), which describes the relative size between particle and hard sphere radii, plays an important role in the study of this two-size model.

Our aim here is to present and study a dynamical version of the AO-model and its depletion feature. We first construct, in Section 2, an infinite-dimensional random diffusion dynamics whose reversible (i.e., equilibrium) measure is the AO-Model for n hard spheres in a bath of infinitely many particles. Section 3 is devoted to the study of the projection of this two-type equilibrium measure onto the subsystem of hard spheres. We first notice how it induces a new attractive interaction (in the sense of Statistical Mechanics) between the hard spheres, called depletion interaction. This new term is induced by the hidden presence of the particle bath and is proportional to the volume of the depletion shells around the hard spheres, see Proposition 3.1. Detailed computations and geometric comments in particular cases are then presented. Moreover, a gradient random dynamics associated to this measure is proposed in Section 3.2. In Section 3.3, we consider the asymptotic regime corresponding to the system of n spheres in a bath with a very high density of particles. The depletion interaction thus dominates the system to the extent that the equilibrium measure concentrates on n -hard-sphere configurations in \mathbb{R}^d which maximise their contact number. In this way, we obtain a constructive random dynamical approach via gradient diffusions to the difficult problem of optimal sphere packing for any number n of spheres and in any dimension d .

In order to get an understanding for the behaviour of the two-type dynamics of Section 2, as well as of the gradient random dynamics with depletion studied in Section 3.2, we decided to write a Python code to generate some simulations. The link to the GitLab page is provided in Section 4, along with a short presentation of the animations one can find there.

2 Diffusion of hard spheres in an infinite bath of Brownian particles

Finding an appropriate random dynamics that describes the time-evolution of various two-type physical systems is an old challenge. See, e.g., the mechanical model of Brownian motion proposed in [8] for the motion of a large component whose velocity follows an Ornstein-Uhlenbeck diffusion in an infinite bath of small particles; [22], in which a Brownian sphere interacts with infinitely-many particles of vanishing radius; [7], in which the authors exhibit a kind of Archimedes' principle for a large disc evolving as a Brownian motion with drift (due to the force of gravity) in a one-sided open cylinder of \mathbb{R}^2 , submerged in a large number of much smaller discs.

Despite the vast literature, to the best of our knowledge, there is no study that takes into account a two-type hard-core interaction. The specificity of our approach lies therefore in the construction of a strong solution to an infinite-dimensional stochastic differential system for a two-size model of large hard spheres and small particles that are diffusing under the infinitely-many non-overlap constraints (1.1). The main technical difficulty consists in controlling the reflection at the boundary of the set of admissible configurations, expressed mathematically as infinitely-many local-time terms appearing in the SDE that describes the time evolution of each sphere.

2.1 Existence and uniqueness result for an infinite-dimensional random dynamics with reflection

We now introduce and study the random evolution in \mathbb{R}^d of our two-type system. To simplify, we restrict the time evolution to the time interval $[0, 1]$, noting that it can be extended by Markovianity to any time interval.

The system is described as follows:

- n hard spheres with radius \mathring{r} , whose centres at time t are denoted by $\{\mathring{X}_1(t), \dots, \mathring{X}_n(t)\}$, move according to n independent Brownian motions.

In order to avoid their dispersion at infinity, they are smoothly confined around the origin by a self-potential $\mathring{\psi} : \mathbb{R}^d \rightarrow \mathbb{R}$ of class C^2 with bounded derivatives and satisfying

$$\int_{\mathbb{R}^d} \exp(-\mathring{\psi}(x)) dx = 1 \quad \text{and} \quad \int_{\mathbb{R}^d} |x|^2 e^{-\mathring{\psi}(x)} dx < +\infty. \quad (2.1)$$

It is simple to show that such a function (having linear growth with respect to the Euclidean norm at infinity) exists. Moreover, the measure

$$\lambda(dx) := \exp(-\mathring{\psi}(x)) dx$$

is a probability measure with second moment, and plays a reference role in what follows.

- The hard spheres evolve in a time-inhomogeneous *random medium* consisting of a field $\sum_k \delta_{\mathring{X}_k(\cdot)}$ of intensity \mathring{z} of infinitely many small particles, themselves moving according to $\mathring{\sigma}$ -scaled independent Brownian motions.
- The only interactions between the hard spheres and the small particles are due to the *non-overlap constraints* (1.1), in the sense that, at each time, the two-type configuration should be admissible.

We can then describe this two-type dynamics with the following infinite-dimensional stochastic differential equation (SDE) with reflection:

$$\left\{ \begin{array}{l} \text{for } i, j \in \{1, \dots, n\}, k \in \mathbb{N}^*, t \in [0, 1], \\ \dot{X}_i(t) = \dot{X}_i(0) + \dot{W}_i(t) - \frac{1}{2} \int_0^t \nabla \dot{\psi}(\dot{X}_i(s)) ds \\ \quad + \sum_{j=1}^n \int_0^t (\dot{X}_i(s) - \dot{X}_j(s)) dL_{ij}(s) + \sum_{k \geq 1} \int_0^t (\dot{X}_i(s) - \dot{X}_k(s)) d\ell_{ik}(s), \\ \dot{X}_k(t) = \dot{X}_k(0) + \dot{W}_k(t) + \dot{\sigma}^2 \sum_{i=1}^n \int_0^t (\dot{X}_k(s) - \dot{X}_i(s)) d\ell_{ki}(s), \\ L_{ij}(0) = 0, \quad L_{ij} \equiv L_{ji}, \quad L_{ij}(t) = \int_0^t \mathbb{1}_{|\dot{X}_i(s) - \dot{X}_j(s)| = 2\hat{r}} dL_{ij}(s), \quad L_{ii} \equiv 0, \\ \ell_{ik}(0) = 0, \quad \ell_{ik} \equiv \ell_{ki}, \quad \ell_{ik}(t) = \int_0^t \mathbb{1}_{|\dot{X}_i(s) - \dot{X}_k(s)| = \hat{r} + \hat{r}} d\ell_{ik}(s), \quad \ell_{ii} \equiv 0, \end{array} \right. \quad (\mathfrak{S})$$

where the i.i.d. sequences of \mathbb{R}^d -valued Brownian motions $(\dot{W}_i)_{i=1, \dots, n}$ and $(\dot{W}_k)_{k \in \mathbb{N}^*}$ are independent.

The local times $(L_{ij})_{i, j \in \{1, \dots, n\}}$ ensure that the hard spheres do not overlap pairwise. In case of collision, they are submitted to an instantaneous repulsion corresponding to a normal reflection at the boundary of the set of admissible configurations. Analogously, the local times $(\ell_{ik})_{i \in \{1, \dots, n\}, k \in \mathbb{N}^*}$ ensure that the small particles do not overlap with the hard spheres.

The gradient term $\nabla \dot{\psi}$ guarantees that, in the absence of small particles, the large spheres undergo a recurrent diffusive motion whose unique reversible probability measure is known. The diffusion coefficient $\dot{\sigma}$ parametrises the mobility of the small particles.

We can now state the main result of this section.

Theorem 2.1. The infinite-dimensional SDE with reflection (\mathfrak{S}) admits for μ -almost every deterministic initial condition a unique \mathcal{D} -valued strong solution. The probability measure μ , concentrated on \mathcal{D} , is given by (2.8).

The rest of this section is devoted to the proof of the above theorem. We split it into four steps, taking inspiration from, and generalising, the existence theorem obtained in [10] for an infinite-dimensional diffusion with reflection of equal (one-size) spheres:

Step 1: *Dynamics for n hard spheres and m confined particles.*

We first approximate the above infinite-dimensional dynamics by a two-type dynamics concerning only a finite number $m \geq 1$ of particles. Moreover, we confine them by adding to their dynamics a restoring gradient drift that prevents their dispersion. The resulting dynamics is then described by the following

finite-dimensional SDE:

$$\left\{ \begin{array}{l} \text{for } i \in \{1, \dots, n\}, k \in \{1, \dots, m\}, t \in [0, 1], \\ \dot{X}_i(t) = \dot{X}_i(0) + \dot{W}_i(t) - \frac{1}{2} \int_0^t \nabla \dot{\psi}(\dot{X}_i(s)) ds \\ \quad + \sum_{j=1}^n \int_0^t (\dot{X}_i - \dot{X}_j)(s) dL_{ij}(s) + \sum_{k'=1}^m \int_0^t (\dot{X}_i - \dot{X}_{k'})(s) d\ell_{ik'}(s), \\ \dot{X}_k(t) = \dot{X}_k(0) + \dot{W}_k(t) - \frac{\dot{\sigma}^2}{2} \int_0^t \nabla \dot{\psi}^R(\dot{X}_i(s)) ds \\ \quad + \dot{\sigma}^2 \sum_{i=1}^n \int_0^t (\dot{X}_k - \dot{X}_i)(s) d\ell_{ki}(s), \\ L_{ij}(0) = 0, \quad L_{ij} \equiv L_{ji}, \quad L_{ij}(t) = \int_0^t \mathbb{1}_{|\dot{X}_i(s) - \dot{X}_j(s)| = 2\hat{r}} dL_{ij}(s), \quad L_{ii} \equiv 0, \\ \ell_{ik}(0) = 0, \quad \ell_{ik} \equiv \ell_{ki}, \quad \ell_{ik}(t) = \int_0^t \mathbb{1}_{|\dot{X}_i(s) - \dot{X}_k(s)| = \hat{r} + \hat{r}} d\ell_{ik}(s), \quad \ell_{ii} \equiv 0. \end{array} \right. \quad (\mathfrak{S}_{m,R})$$

where $\dot{W}_i, 1 \leq i \leq n, \dot{W}_k, 1 \leq k \leq m$, are independent \mathbb{R}^d -valued Brownian motions.

The function $\dot{\psi}^R : \mathbb{R}^d \mapsto \mathbb{R}_+$ confining the particles is of class C^2 with bounded derivatives. Moreover, it depends on the parameter $R \in \mathbb{N}$ in the following way:

$$\dot{\psi}^R(x) = 0 \text{ if } x \in B(0, R) \quad \text{and} \quad \sum_{R=1}^{\infty} \int_{B(0,R)^c} e^{-\dot{\psi}^R(x)} dx < +\infty. \quad (2.2)$$

Since it vanishes in the ball $B(0, R)$, its confining effect decreases and eventually disappears as R tends to infinity. Such a function can be constructed, e.g., by defining it proportional to $|x| - R$ for x far from the origin.

We define the set of *finite* admissible configurations with m particles as $\mathcal{D}_m := \mathcal{D} \cap \mathcal{M}_m$.

Proposition 2.2. The SDE with reflection $(\mathfrak{S}_{m,R})$ admits, for any deterministic initial condition in the interior of the domain \mathcal{D}_m , a unique strong solution

$$(\dot{X}_i^{m,R}(t), \dot{X}_k^{m,R}(t), L_{ij}^{m,R}(t), \ell_{ik}^{m,R}(t))_{t \in [0,1], 1 \leq i,j \leq n, 1 \leq k \leq m}.$$

The finite measure $\nu^{m,R}$, concentrated on the admissible configurations with m particles, and given by

$$\nu^{m,R}(d\mathbf{x}) := \mathbb{1}_{\mathcal{D}_m}(\mathbf{x}) e^{-\sum_{k=1}^m \dot{\psi}^R(\dot{x}_k)} \otimes_{i=1}^n \lambda(d\dot{x}_i) \otimes_{k=1}^m d\dot{x}_k, \quad (2.3)$$

where $\mathbf{x} = \{\dot{x}_1, \dots, \dot{x}_n, \dot{x}_1, \dots, \dot{x}_m\}$, is reversible for the dynamics $(\mathfrak{S}_{m,R})$.

Remark 2.3. Due to the assumptions (2.2) satisfied by the confining potential $\dot{\psi}^R$, the measure $\nu^{m,R}$ is mainly supported on configurations whose m particles are in the ball $B(0, R)$ (or close to that ball). Moreover, the integral $\int_{\mathbb{R}^d} e^{-\dot{\psi}^R(x)} dx$ is finite and increases at most polynomially in R when R tends to infinity.

Proof of Proposition 2.2. The system $(\mathfrak{S}_{m,R})$ describes the dynamics of an $(n + m)d$ -dimensional gradient diffusion with reflection at the boundary of the domain \mathcal{D}_m . The different size of the hard spheres and the particles induces a new geometric complexity which did not exist in the case of identical spheres studied in [10].

In [9], the first author solved the question of existence and uniqueness of a reflected diffusion in a geometric domain whose boundary is induced by several constraints. There, the required assumptions are (i) a regularity condition on each constraint; and (ii) a so-called *compatibility* condition between the constraints. We check here that the domain $\mathcal{D}_m \subset \mathcal{M}_m$ satisfies such properties, as stated in [9, Definition 2.1].

The interior of the domain \mathcal{D}_m can be described as the following intersection of sets:

$$\text{int}(\mathcal{D}_m) = \bigcap_{\substack{1 \leq i, j \leq n \\ j \neq i}} \left\{ \mathbf{x} \in \mathcal{M}_m : \Gamma_{ij}(\mathbf{x}) > 0 \right\} \cap \bigcap_{\substack{1 \leq i \leq n \\ 1 \leq k \leq m}} \left\{ \mathbf{x} \in \mathcal{M}_m : \gamma_{ik}(\mathbf{x}) > 0 \right\}.$$

The C^2 constraint function

$$\Gamma_{ij}(\mathbf{x}) = \Gamma_{ij}(\overset{\circ}{\mathbf{x}}) := \frac{|\overset{\circ}{x}_i - \overset{\circ}{x}_j|^2}{4\overset{\circ}{r}^2} - 1 \quad (2.4)$$

controls the distance between the hard spheres i and j , whereas the C^2 constraint function

$$\gamma_{ik}(\mathbf{x}) := \frac{|\overset{\circ}{x}_i - \overset{\circ}{x}_k|^2}{\overset{\circ}{r}^2} - 1$$

controls the distance between the hard sphere i and the particle k . The boundary of \mathcal{D}_m is then a union of smooth boundaries, each one being the set of zeros of one constraint.

(i) *Boundedness of first and second derivatives of the constraint functions.*

We first prove that the norm of the gradient of each constraint function is uniformly bounded from below on its induced boundary.

It is straightforward to check that, for $\mathbf{x} = \{\overset{\circ}{x}_1, \dots, \overset{\circ}{x}_n, \overset{\circ}{x}_1, \dots, \overset{\circ}{x}_m\}$,

- if $\Gamma_{ij}(\mathbf{x}) = 0$, i.e., $|\overset{\circ}{x}_i - \overset{\circ}{x}_j|^2 = 4\overset{\circ}{r}^2$, then $|\nabla \Gamma_{ij}(\mathbf{x})|^2 = 8|\overset{\circ}{x}_i - \overset{\circ}{x}_j|^2/16\overset{\circ}{r}^4 = 2/\overset{\circ}{r}^2 > 0$;
- if $\gamma_{ik}(\mathbf{x}) = 0$, i.e., $|\overset{\circ}{x}_i - \overset{\circ}{x}_k|^2 = \overset{\circ}{r}^2$ then $|\nabla \gamma_{ik}(\mathbf{x})|^2 = 8/\overset{\circ}{r}^2 > 0$.

Second derivatives are uniformly bounded from above because they are constant.

(ii) *Compatibility between the constraints.*

We are now looking for a positive constant b_0 such that, at any point \mathbf{x} of the ij -boundary (resp. ik -boundary) of \mathcal{D}_m , there exists a non-zero vector $\mathbf{v} \in (\mathbb{R}^d)^{n+m}$, such that

$$\mathbf{v} \cdot \nabla \Gamma_{ij}(\mathbf{x}) \geq b_0 |\mathbf{v}| |\nabla \Gamma_{ij}(\mathbf{x})| \quad (\text{resp. } \mathbf{v} \cdot \nabla \gamma_{ik}(\mathbf{x}) \geq b_0 |\mathbf{v}| |\nabla \gamma_{ik}(\mathbf{x})|).$$

More precisely, if a configuration $\mathbf{x} = \overset{\circ}{\mathbf{x}}\overset{\circ}{\mathbf{x}}$ belongs, e.g., to the ij -boundary, the hard spheres i and j collide. Heuristically, the vector \mathbf{v} indicates the most effective impulse for the configuration to come back into the interior of the domain \mathcal{D}_m , i.e., for the colliding spheres to go away from each other as fast as possible. The compatibility condition requires that the maximum angle between all these impulses, which is equal to $2 \arccos b_0$, remains bounded away from π .

Fix $\mathbf{x} \in \partial \mathcal{D}_m$, and let $C(\overset{\circ}{x}_i)$ be the cluster around the i -th sphere $\overset{\circ}{x}_i$ (resp. $C(\overset{\circ}{x}_k)$ the cluster around the k -th particle $\overset{\circ}{x}_k$), that is, the set of all spheres or particles of \mathbf{x} either touching $\overset{\circ}{x}_i$ or belonging to a chain of spheres and/or particles in contact including $\overset{\circ}{x}_i$ (similarly for $\overset{\circ}{x}_k$). We define the centre of mass of such clusters by

$$\mathbf{m}(\overset{\circ}{x}_i) := \frac{1}{\#C(\overset{\circ}{x}_i)} \sum_{x_j \in C(\overset{\circ}{x}_i)} x_j \quad \text{and} \quad \mathbf{m}(\overset{\circ}{x}_k) := \frac{1}{\#C(\overset{\circ}{x}_k)} \sum_{x_j \in C(\overset{\circ}{x}_k)} x_j$$

and the vector $\mathbf{v} = \overset{\circ}{\mathbf{v}} \overset{\circ}{\mathbf{v}} \in \mathbb{R}^{dn} \times \mathbb{R}^{dm}$ by

$$\overset{\circ}{v}_i := \overset{\circ}{x}_i - \mathbf{m}(\overset{\circ}{x}_i) \quad \text{and} \quad \overset{\circ}{v}_k := \overset{\circ}{x}_k - \mathbf{m}(\overset{\circ}{x}_k).$$

It is not difficult to show that

$$\Gamma_{ij}(\mathbf{x}) = 0 \Rightarrow \mathbf{v} \cdot \frac{\nabla \Gamma_{ij}(\mathbf{x})}{|\nabla \Gamma_{ij}(\mathbf{x})|} = \sqrt{2} \overset{\circ}{r} \quad \text{and} \quad \gamma_{ik}(\mathbf{x}) = 0 \Rightarrow \mathbf{v} \cdot \frac{\nabla \gamma_{ik}(\mathbf{x})}{|\nabla \gamma_{ik}(\mathbf{x})|} = \frac{\overset{\circ}{r}}{\sqrt{2}}.$$

Moreover, $|\mathbf{v}|^2 \leq 4\overset{\circ}{r}^2(n+m)^3$. Therefore, one can choose $b_0 := \frac{\overset{\circ}{r}}{2\sqrt{2}\overset{\circ}{r}(n+m)^{3/2}} > 0$.

Note that b_0 vanishes as m tends to infinity. Therefore this method to prove existence cannot be applied to the case $m = +\infty$.

Having proved that the constraints defining the domain \mathcal{D}_m are compatible in the sense of [9], we can now apply Theorem 2.2 therein, yielding the existence and uniqueness, for each initial admissible configuration, of a strong solution to the SDE with reflection $(\mathfrak{S}_{m,R})$.

Its diffusion matrix is the $(d(n+m) \times d(n+m))$ -block matrix of diagonal matrices $\begin{pmatrix} I_{nd} & 0 \\ 0 & \overset{\circ}{\sigma} I_{md} \end{pmatrix}$ and its drift is given by the gradient of the potential function $\Phi(\mathbf{x}) := \sum_{i=1}^n \overset{\circ}{\psi}(\overset{\circ}{x}_i) + \sum_{k=1}^m \overset{\circ}{\psi}^R(\overset{\circ}{x}_k)$.

Applying [9, Theorem 2.5] (see also [21]), we get that $\mathbb{1}_{\mathcal{D}_m}(\mathbf{x})e^{-\Phi(\mathbf{x})}d\mathbf{x}$ is a time-reversible measure for the dynamics $(\mathfrak{S}_{m,R})$. This concludes the proof of the proposition. \square

Step 2: Localisation of the initial particles.

We consider again the finite-dimensional dynamics $(\mathfrak{S}_{m,R})$, and fit the number m of particles to the confinement parameter R in the following way. Let $\mathbf{x} = \overset{\circ}{\mathbf{x}} \overset{\circ}{\mathbf{x}} \in \mathcal{D}$ be an admissible configuration; we define the finite-dimensional process

$$X^{\mathbf{x},R} = \left(\overset{\circ}{X}_i^{\mathbf{x},R}(t), \overset{\circ}{X}_k^{\mathbf{x},R}(t), L_{ij}^{\mathbf{x},R}(t), \ell_{ik}^{\mathbf{x},R}(t) \right)_{t \in [0,1], 1 \leq i,j \leq n, 1 \leq k \leq m} \quad (2.5)$$

as the solution of the SDE $(\mathfrak{S}_{m,R})$ with initial condition $\overset{\circ}{\mathbf{x}}$ for the n hard spheres and $\overset{\circ}{\mathbf{x}}_{|_R}$ for the particles, where $\overset{\circ}{\mathbf{x}}_{|_R}$ denotes the subset of particles in $\overset{\circ}{\mathbf{x}}$ which belong to the ball $B(0, R)$. Therefore the corresponding dimension $m = m(\overset{\circ}{\mathbf{x}}, R)$ is equal to the finite number $\#\overset{\circ}{\mathbf{x}}_{|_R}$ of particles.

For any continuous function $f: [0, 1] \rightarrow \mathbb{R}^d$, let w be its *modulus of continuity*, that is for any $\delta > 0$, $w(f, \delta) := \sup\{|f(t) - f(s)|, |t - s| < \delta\}$. We say that a continuous path is *nice* if it stays away from the origin, or if its modulus of continuity w is bounded. More precisely, for any $\alpha, \delta, \varepsilon > 0$, we define the set of $(\alpha, \delta, \varepsilon)$ -*nice paths* as

$$\mathcal{N}(\alpha, \delta, \varepsilon) := \left\{ f: [0, 1] \rightarrow \mathbb{R}^d \text{ continuous s.t. } \min_{s \in [0,1]} |f(s)| > \alpha \text{ or } w(f, \delta) \leq \varepsilon \right\}. \quad (2.6)$$

Finally, for $\mathbf{x} \in \mathcal{D}$, we define an event $\Omega_{\mathbf{x}} \subset \Omega$, on which we will be able to construct the solution of

the infinite dimensional two-type dynamics (\mathfrak{S}) , as follows:

$$\begin{aligned} \Omega_{\mathbf{x}} := & \left\{ \omega \in \Omega : \forall \mathring{R} \in \mathbb{N}^* \exists \mathring{R} \in \mathbb{N}^* \forall R \geq \mathring{R}, \right. \\ & \forall i \leq n, \dot{X}_i^{\mathbf{x},R}(\omega) \in \mathcal{N}(\mathring{R} + \sqrt{R}, \frac{1}{\sqrt{R}}, 1), \\ & \forall k \leq m(\dot{\mathbf{x}}, R), \dot{X}_k^{\mathbf{x},R}(\omega) \in \mathcal{N}(\mathring{R} + \mathring{r} + \sqrt{R}, \frac{1}{\sqrt{R}}, 1), \\ & \forall i \leq n, \dot{X}_i^{\mathbf{x},R+1}(\omega) \in \mathcal{N}(\mathring{R} + \sqrt{R}, \frac{1}{\sqrt{R}}, 1), \\ & \left. \forall k \leq m(\dot{\mathbf{x}}, R+1), \dot{X}_k^{\mathbf{x},R+1}(\omega) \in \mathcal{N}(\mathring{R} + \mathring{r} + \sqrt{R}, \frac{1}{\sqrt{R}}, 1) \right\}. \end{aligned} \quad (2.7)$$

Step 3: Convergence on $\Omega_{\mathbf{x}} \subset \Omega$ of the approximating processes.

Proposition 2.4. Fix \mathbf{x} in \mathcal{D} . The sequence $(X^{\mathbf{x},R}(\omega), \omega \in \Omega_{\mathbf{x}})_{R \in \mathbb{N}^*}$ defined in (2.5) converges to a limit process denoted by $X^{\mathbf{x}} := \left(\dot{X}_i^{\mathbf{x}}, \dot{X}_k^{\mathbf{x}}, L_{ij}^{\mathbf{x}}, \ell_{ik}^{\mathbf{x}} \right)_{1 \leq i, j \leq n, k \geq 1}$. This process is solution on $\Omega_{\mathbf{x}}$ of the infinite-dimensional equation (\mathfrak{S}) with initial configuration \mathbf{x} .

Proof. Fix $\mathbf{x} = \dot{\mathbf{x}} \in \mathcal{D}$ and $\omega \in \Omega_{\mathbf{x}}$.

We first prove that, for fixed $1 \leq i, j \leq n$ and $k \in \mathbb{N}^*$, the four sequences

$$\left(\dot{X}_i^{\mathbf{x},R}(\omega) \right)_R, \left(\dot{X}_k^{\mathbf{x},R}(\omega) \right)_R, \left(L_{ij}^{\mathbf{x},R}(\omega) \right)_R, \left(\ell_{ik}^{\mathbf{x},R}(\omega) \right)_R$$

are eventually constant. Choose $\mathring{R} := \lceil \max\{|\dot{x}_i|, 1 \leq i \leq n\} \rceil$ ($\lceil z \rceil$ denotes the smallest integer larger than $z \in \mathbb{R}$). The initial position \dot{x}_i of the i -th hard-sphere centre belongs therefore to $B(0, \mathring{R})$.

Since both paths $\dot{X}_i^{\mathbf{x},R}(\omega)$ and $\dot{X}_i^{\mathbf{x},R+1}(\omega)$ belong to the set $\mathcal{N}(\mathring{R} + \sqrt{R}, 1/\sqrt{R}, 1)$, then

$$w(\dot{X}_i^{\mathbf{x},R}(\omega), 1/\sqrt{R}) \leq 1 \text{ as soon as } \min_{t \in [0,1]} |\dot{X}_i^{\mathbf{x},R}(\omega, t)| \leq \mathring{R} + \sqrt{R},$$

and the same holds for $\dot{X}_i^{\mathbf{x},R+1}(\omega)$.

Moreover, since a path with δ -modulus of continuity bounded by ε started in $B(0, \alpha)$ remains in $B(0, \alpha + \frac{\varepsilon}{\delta})$ for the time interval $[0, 1]$ then, taking $\alpha = \mathring{R}$, $\delta = 1/\sqrt{R}$ and $\varepsilon = 1$, then

$$\max_{t \in [0,1]} |\dot{X}_i^{\mathbf{x},R}(\omega, t)| \leq \mathring{R} + \sqrt{R} \text{ as soon as } \min_{t \in [0,1]} |\dot{X}_i^{\mathbf{x},R}(\omega, t)| \leq \mathring{R} + \sqrt{R}.$$

This is indeed the case, as the above condition is always satisfied, since

$$\min_{t \in [0,1]} |\dot{X}_i^{\mathbf{x},R}(\omega, t)| \leq |\dot{X}_i^{\mathbf{x},R}(\omega, 0)| \leq \mathring{R}.$$

The same argument holds for $\dot{X}_i^{\mathbf{x},R+1}(\omega)$.

This implies in particular that every particle $\dot{X}_k^{\mathbf{x},R}(\omega)$ which collides with some hard sphere $\dot{X}_i^{\mathbf{x},R}(\omega)$ belongs to $B(0, \mathring{R} + \mathring{r} + \sqrt{R})$ at the time of the collision.

Since the path $\dot{X}_k^{\mathbf{x},R}(\omega)$ belongs to $\mathcal{N}(\mathring{R} + \mathring{r} + \sqrt{R}, 1/\sqrt{R}, 1)$, if it collides with some hard sphere, its $(1/\sqrt{R})$ -modulus of continuity is bounded by 1. The same argument holds for $\dot{X}_k^{\mathbf{x},R+1}(\omega)$.

So, since particles that collide with a hard sphere at some time $t \in [0, 1]$ cannot cover more than a distance \sqrt{R} during the time interval $[0, 1]$, their paths stay in the ball $B(0, \mathring{R} + \mathring{r} + 2\sqrt{R})$.

As a consequence, for R large enough in the sense that $R \geq \mathring{R} + \mathring{r} + 2\sqrt{R}$ (this holds as soon as $R \geq \underline{R} := 4 + 2(\mathring{R} + \mathring{r})$), the hard spheres and the particles that visit $B(0, \mathring{R} + \mathring{r} + \sqrt{R})$ stay in a region where the self-potentials $\dot{\psi}^R$ and $\dot{\psi}^{R+1}$ vanish. That is, the k -th-particle dynamics computed at ω in $(\mathfrak{S}_{m,R})$ does not feel $\dot{\psi}^R$ if it collides with hard spheres or if it starts in $B(0, \mathring{R} + \mathring{r} + \sqrt{R})$. Consequently, the sphere dynamics computed at ω in both equations $(\mathfrak{S}_{m,R})$ and $(\mathfrak{S}_{m,R+1})$ coincide when $R \geq \underline{R}$, and the k -th-particle dynamics computed at ω coincide as soon as $\dot{x}_k \in B(0, \mathring{R} + \mathring{r} + \sqrt{R})$.

The strong uniqueness in Theorem 2.2 of [9] allows us to deduce the existence of paths $\dot{X}_i^{\mathbf{x}}(\omega)$, $\dot{X}_k^{\mathbf{x}}(\omega)$, $L_{ij}^{\mathbf{x}}(\omega)$ and $\ell_{ik}^{\mathbf{x}}(\omega)$ such that

$$\forall R \geq \underline{R}, \forall 1 \leq i, j \leq n, \forall k \text{ such that } \dot{x}_k \in B(0, \mathring{R} + \mathring{r} + \sqrt{R}), \forall t \in [0, 1],$$

$$\dot{X}_i^{\mathbf{x},R}(\omega, t) = \dot{X}_i^{\mathbf{x}}(\omega, t), \dot{X}_k^{\mathbf{x},R}(\omega, t) = \dot{X}_k^{\mathbf{x}}(\omega, t), L_{ij}^{\mathbf{x},R}(\omega, t) = L_{ij}^{\mathbf{x}}(\omega, t), \ell_{ik}^{\mathbf{x},R}(\omega, t) = \ell_{ik}^{\mathbf{x}}(\omega, t).$$

By construction then, these paths satisfy the following SDE

$$\left\{ \begin{array}{l} \text{for } i \in \{1, \dots, n\}, k \in \mathbb{N}^*, t \in [0, 1], \\ \dot{X}_i^{\mathbf{x}}(\omega, t) = \dot{x}_i + \dot{W}_i(\omega, t) - \frac{1}{2} \int_0^t \nabla \dot{\psi}(\dot{X}_i^{\mathbf{x}}(\omega, s)) ds \\ \quad + \sum_{j=1}^n \int_0^t (\dot{X}_i^{\mathbf{x}}(\omega, s) - \dot{X}_j^{\mathbf{x}}(\omega, s)) dL_{ij}^{\mathbf{x}}(\omega, s) \\ \quad + \sum_{k'=1}^{+\infty} \int_0^t (\dot{X}_i^{\mathbf{x}}(\omega, s) - \dot{X}_{k'}^{\mathbf{x}}(\omega, s)) d\ell_{ik'}^{\mathbf{x}}(\omega, s), \\ \dot{X}_k^{\mathbf{x}}(\omega, t) = \dot{x}_k + \dot{\sigma} \dot{W}_k(\omega, t) + \dot{\sigma}^2 \sum_{i=1}^n \int_0^t (\dot{X}_k^{\mathbf{x}}(\omega, s) - \dot{X}_i^{\mathbf{x}}(\omega, s)) d\ell_{ki}^{\mathbf{x}}(\omega, s), \\ L_{ij}^{\mathbf{x}}(\omega, 0) = 0, \quad L_{ij}^{\mathbf{x}} \equiv L_{ji}^{\mathbf{x}}, \quad L_{ij}^{\mathbf{x}}(\omega, t) = \int_0^t \mathbb{1}_{|\dot{X}_i^{\mathbf{x}}(\omega, s) - \dot{X}_j^{\mathbf{x}}(\omega, s)| = 2\mathring{r}} dL_{ij}^{\mathbf{x}}(\omega, s), \quad L_{ii}^{\mathbf{x}} \equiv 0, \\ \ell_{ik}^{\mathbf{x}}(\omega, 0) = 0, \quad \ell_{ik}^{\mathbf{x}} \equiv \ell_{ki}^{\mathbf{x}}, \quad \ell_{ik}^{\mathbf{x}}(\omega, t) = \int_0^t \mathbb{1}_{|\dot{X}_i^{\mathbf{x}}(\omega, s) - \dot{X}_k^{\mathbf{x}}(\omega, s)| = \mathring{r}} d\ell_{ik}^{\mathbf{x}}(\omega, s), \quad \ell_{ii}^{\mathbf{x}} \equiv 0. \end{array} \right.$$

This concludes the proof. \square

Step 4: *The constructed solution of (\mathfrak{S}) is defined on a full subset of Ω .*

We first introduce a probability measure μ on the set of admissible configurations \mathcal{D} , as the law of n free hard spheres – each one submitted to the self-potential $\dot{\psi}$ – in an admissible Poisson bath of particles. In Section 2.2 we will eventually prove that μ is indeed the reversible probability measure for the dynamics (\mathfrak{S}) .

Let $\pi(d\dot{\mathbf{x}})$ denote the Poisson point process on $\dot{\mathcal{M}}$ with intensity $\dot{z} > 0$, where \dot{z} is a fixed parameter (we let vary it only in the last section of the paper). We consider the following probability measure μ on \mathcal{M} with support in \mathcal{D} :

$$\mu(d\mathbf{x}) = \frac{1}{Z} \mathbb{1}_{\mathcal{D}}(\dot{\mathbf{x}}\dot{\mathbf{x}}) \pi(d\dot{\mathbf{x}}) * \delta_{\dot{\mathbf{x}}} \otimes_{i=1}^n \lambda(d\dot{x}_i), \quad \mathbf{x} = \dot{\mathbf{x}}\dot{\mathbf{x}}.$$

The normalisation constant

$$Z = \int_{\mathcal{M}} \mathbb{1}_{\mathcal{D}}(\dot{\mathbf{x}}\dot{\mathbf{x}}) \pi(d\dot{\mathbf{x}}) \otimes_{i=1}^n \lambda(d\dot{x}_i) < +\infty$$

is finite since the measure λ has finite mass.

Notice that, by considering $\otimes_{i=1}^n \lambda(d\dot{x}_i)$ we have enforced an ordering on the hard spheres $\dot{\mathbf{x}}$. It should be multiplied by $1/n!$, but this factor is absorbed by the normalisation constant Z .

Equivalently, μ is characterised as follows: for any positive measurable function F on \mathcal{D} ,

$$\int_{\mathcal{D}} F(\mathbf{x}) \mu(d\mathbf{x}) := \frac{1}{Z} \int_{\mathbb{R}^{nd}} \int_{\dot{\mathcal{M}}} F(\dot{\mathbf{x}}\dot{\mathbf{x}}) \mathbb{1}_{\mathcal{D}}(\dot{\mathbf{x}}\dot{\mathbf{x}}) \pi(d\dot{\mathbf{x}}) \otimes_{i=1}^n \lambda(d\dot{x}_i). \tag{2.8}$$

Proposition 2.5. For μ -a.e. $\mathbf{x} \in \mathcal{D}$,

$$P(\Omega_{\mathbf{x}}) = 1.$$

Therefore, the limit process $X^{\mathbf{x}}$ constructed in Proposition 2.4 is well defined for μ -almost every initial configuration \mathbf{x} .

Proof. We aim to prove that $\int_{\mathcal{D}} P((\Omega_{\mathbf{x}})^c) d\mu(\mathbf{x}) = 0$.

Due to the definition of $\Omega_{\mathbf{x}}$ given in (2.7), we can write its complement set $(\Omega_{\mathbf{x}})^c$ as

$$\bigcup_{\dot{R} \in \mathbb{N}^*} \limsup_R \left\{ \exists i \leq n : \dot{X}_i^{\mathbf{x},R} \in \mathcal{B}(\dot{R} + \sqrt{R}, \frac{1}{\sqrt{R}}, 1) \cup \mathcal{B}(\dot{R} + \sqrt{R-1}, \frac{1}{\sqrt{R-1}}, 1) \text{ or} \right. \\ \left. \exists k \leq m(\dot{\mathbf{x}}, R) : \dot{X}_k^{\mathbf{x},R} \in \mathcal{B}(\dot{R} + \overset{\circ}{r} + \sqrt{R}, \frac{1}{\sqrt{R}}, 1) \cup \mathcal{B}(\dot{R} + \sqrt{R-1}, \frac{1}{\sqrt{R-1}}, 1) \right\},$$

where \mathcal{B} denotes the set of *bad paths*, complement of the set \mathcal{N} of nice paths defined in (2.6):

$$\mathcal{B}(\alpha, \delta, \varepsilon) := \left\{ f : [0, 1] \rightarrow \mathbb{R}^d \text{ continuous s.t. } \min_{s \in [0,1]} |f(s)| \leq \alpha \text{ and } w(f, \delta) > \varepsilon \right\}.$$

In other words, a path in $\mathcal{B}(\alpha, \delta, \varepsilon)$ visits the ball $B(0, \alpha)$ during the time interval $[0, 1]$ and its δ -modulus of continuity is larger than ε .

Since $\mathcal{B}(\alpha, \delta, \varepsilon)$ increases as α increases and increases as δ increases, it suffices to prove that

$$\int_{\mathcal{D}} P(\tilde{\Omega}_{\mathbf{x}}) d\mu(\mathbf{x}) = 0, \text{ where}$$

$$\tilde{\Omega}_{\mathbf{x}} := \bigcup_{\dot{R} \in \mathbb{N}^*} \limsup_R \left\{ \exists i \leq n : \dot{X}_i^{\mathbf{x},R} \in \mathcal{B}(\dot{R} + \sqrt{R}, \frac{1}{\sqrt{R-1}}, 1) \right. \\ \left. \text{or } \exists k \leq m(\dot{\mathbf{x}}, R) : \dot{X}_k^{\mathbf{x},R} \in \mathcal{B}(\dot{R} + \overset{\circ}{r} + \sqrt{R}, \frac{1}{\sqrt{R-1}}, 1) \right\} \supset (\Omega_{\mathbf{x}})^c.$$

Thanks to the Borel–Cantelli lemma, it is then sufficient to prove that, for any $\dot{R} \in \mathbb{N}^*$,

$$\sum_{\dot{R} \in \mathbb{N}^*} \int_{\mathcal{D}} P\left(\exists i \leq n, \dot{X}_i^{\mathbf{x},R} \in \mathcal{B}(\dot{R} + \sqrt{R}, \frac{1}{\sqrt{R-1}}, 1) \text{ or} \right. \\ \left. \exists k \leq m(\dot{\mathbf{x}}, R), \dot{X}_k^{\mathbf{x},R} \in \mathcal{B}(\dot{R} + \overset{\circ}{r} + \sqrt{R}, \frac{1}{\sqrt{R-1}}, 1) \right) d\mu(\mathbf{x}) < +\infty. \tag{2.9}$$

The convergence of the above series will derive from a precise control of the probability of bad paths under various reversible dynamics, which is contained in Lemmas 2.6 and 2.7 below.

Lemma 2.6. Let $\bar{\nu}^{m,R}$ denote the probability measure on \mathcal{D}_m obtained by normalising the measure $\nu^{m,R}$ defined in (2.3).

The reversible solution $X^{m,R}$ of the SDE $(\mathfrak{S}_{m,R})$ with initial distribution $\bar{\nu}^{m,R}$ satisfies the following inequality: for $0 < \alpha < \alpha'$, $\delta \in (0, 1)$ and $\varepsilon > 0$,

$$P_{\bar{\nu}^{m,R}} \left(\exists i \leq n, \dot{X}_i^{m,R} \in \mathcal{B}(\alpha, \delta, \varepsilon) \text{ or } \exists k \leq m, \dot{X}_k^{m,R} \in \mathcal{B}(\alpha', \delta, \varepsilon) \right) \leq \frac{c_1}{\delta} \frac{n+m}{1 - e^{c_0 \delta \alpha^2}} e^{-c_0 \varepsilon^2 / \delta},$$

where $c_0 > 0$ and $c_1 > 0$ are constants depending only on the dimension d and the parameter σ .

For the sake of readability, the proof of this lemma is stated at the end of the section.

Consider now a Poissonian randomisation of the number m of moving particles in the measure $\nu^{m,R}$. It leads to the definition of the following probability measure on \mathcal{D} , mixture of $\nu^{m,R}$ measures :

$$\mu^R := \frac{1}{\mathcal{Z}_R} \sum_{m=0}^{+\infty} \frac{z^m}{m!} \nu^{m,R}, \tag{2.10}$$

where the normalisation constant \mathcal{Z}_R is given by

$$\mathcal{Z}_R = \int_{\mathbb{R}^{dn}} \mathbf{1}_{\mathcal{D}}(\dot{\mathbf{x}}) \exp \left(z \int_{\mathbb{R}^d \setminus \mathbb{B}(\dot{\mathbf{x}})} e^{-\psi^R(x)} dx \right) \otimes_{i=1}^n \lambda(d\dot{x}_i).$$

Recall (see (1.3)) that the interior of the set $\mathbb{B}(\dot{\mathbf{x}}) \subset \mathbb{R}^d$ is the forbidden volume for the centres of particles around the configuration $\dot{\mathbf{x}}$.

By arguments similar to those used in the proof of Lemma 2.6, we can also control the probability that the solution of $(\mathfrak{S}_{m,R})$ with initial distribution μ^R contains bad paths:

Lemma 2.7. The solution of the SDE $(\mathfrak{S}_{m,R})$ with initial distribution μ^R satisfies the following inequality: for $0 < \alpha < \alpha'$, $\delta \in (0; 1)$ and $\varepsilon > 0$,

$$\begin{aligned} P_{\mu^R} \left(\exists i \leq n : \dot{X}_i^{m,R} \in \mathcal{B}(\alpha, \delta, \varepsilon) \text{ or } \exists k \leq m : \dot{X}_k^{m,R} \in \mathcal{B}(\alpha', \delta, \varepsilon) \right) \\ \leq \frac{c_1}{\delta} \left(n + z \int_{\mathbb{R}^d} e^{-\psi^R(x)} dx \right) \frac{e^{-c_0 \varepsilon^2 / \delta}}{1 - e^{c_0 \delta \alpha^2}}, \end{aligned}$$

where $c_0 > 0$ and $c_1 > 0$ are universal constants depending only on the dimension d and the parameter σ .

From Lemma 2.7, together with Remark 2.3, it is now easy to obtain the convergence of the following series:

$$\begin{aligned} \sum_R P_{\mu^R} \left(\exists i \leq n : \dot{X}_i^{m,R} \in \mathcal{B}(\overset{\circ}{R} + \sqrt{R}, \frac{1}{\sqrt{R-1}}, 1) \text{ or} \right. \\ \left. \exists k \leq m : \dot{X}_k^{m,R} \in \mathcal{B}(\overset{\circ}{R} + \overset{\circ}{r} + \sqrt{R}, \frac{1}{\sqrt{R-1}}, 1) \right) \\ \leq \sum_R c_1 \sqrt{R-1} \frac{n + z \int_{\mathbb{R}^d} e^{-\psi^R(x)} dx}{1 - \exp(-c_0(\overset{\circ}{R} + \sqrt{R})^2 / \sqrt{R-1})} e^{-c_0 \sqrt{R-1}} < +\infty. \end{aligned} \tag{2.11}$$

This is still not exactly the summability (2.9) we are aiming for, but we are close.

In order to conclude, we have to compare the two processes below, whose dynamics are given by the same SDE $(\mathfrak{S}_{m,R})$, $m \in \mathbb{N}$, but with different initial distributions:

- The process $X^{m,R}$, with random m and initial configuration $X^{m,R}(0)$ chosen according to the probability measure μ^R , introduced in (2.10);
- The process $X^{\dot{\mathbf{x}},R}$, whose initial configuration $\dot{\mathbf{x}}$ is chosen according to the probability measure μ . In particular, the random number $m = m(\dot{\mathbf{x}}, R)$ corresponds to the number $\#\dot{\mathbf{x}}|_R$ of particles of $\dot{\mathbf{x}}$ in $B(0, R)$, see (2.5).

Note that the first process is reversible – as it is given by a mixture of reversible processes – while the second one is not, since, e.g., its initial law only weighs configuration of particles concentrated in $B(0, R)$.

In order to estimate the difference between these two processes, we consider the total variation distance between their laws, denoted by $\mathbf{d}_{TV}(R)$. It is defined as usual as the supremum over all measurable sets A of continuous paths with values in \mathcal{D} :

$$\begin{aligned} \mathbf{d}_{TV}(R) &:= \sup_{A \subset C([0,1], \mathcal{D})} \left| \int_{\mathcal{D}} P(X^{\#\dot{\mathbf{x}},R} \in A | X^{\#\dot{\mathbf{x}},R}(0) = \mathbf{x}) \mu^R(d\mathbf{x}) \right. \\ &\quad \left. - \int_{\mathcal{D}} P(X^{m(\dot{\mathbf{x}},R),R} \in A | X^{m(\dot{\mathbf{x}},R),R}(0) = \mathbf{x}) \mu(d\mathbf{x}) \right| \\ &= \sup_{A \subset C([0,1], \mathcal{D})} \left| \int_{\mathcal{D}} F_A(\mathbf{x}) \mu^R(d\mathbf{x}) - \int_{\mathcal{D}} F_A(\dot{\mathbf{x}}|_R) \mu(d\mathbf{x}) \right|, \end{aligned}$$

where, for any $m \geq 0$, the function F_A is defined on \mathcal{D}_m by $F_A(\mathbf{x}) := P(X^{m,R} \in A | X^{m,R}(0) = \mathbf{x})$.

In the second integral, we can disintegrate the Poisson point measure π (which models the law of the particles under μ) into the product of the Poisson point measure $\pi|_R$ inside $B(0, R)$ and the Poisson point measure $\pi|_{R^c}$ outside $B(0, R)$. Denoting

$$Z_R := \int_{\dot{\mathcal{M}}} \int_{\mathbb{R}^{dn}} \mathbb{1}_{\mathcal{D}}(\dot{\mathbf{x}}\dot{\mathbf{y}}) e^{z|B(0,R) \setminus \mathbb{B}(\dot{\mathbf{x}})|} \otimes_{i=1}^n \lambda(d\dot{x}_i) d\pi|_{R^c}(\dot{\mathbf{y}}),$$

we then obtain that $\mathbf{d}_{TV}(R)$ is the supremum over A of the following expression:

$$\begin{aligned} &\left| \frac{1}{Z_R} \int_{\mathbb{R}^{dn}} \mathbb{1}_{\mathcal{D}}(\dot{\mathbf{x}}) (F_A(\dot{\mathbf{x}}) \right. \\ &\quad \left. + \sum_{m=1}^{+\infty} \frac{z^m}{m!} \int_{\mathbb{R}^{dm}} F_A(\dot{\mathbf{x}}\dot{x}_1 \dots \dot{x}_m) \prod_{k=1}^m (\mathbb{1}_{\dot{x}_k \notin \mathbb{B}(\dot{\mathbf{x}})} e^{-\psi^R(\dot{x}_k)} \otimes_{k=1}^m d\dot{x}_k) \otimes_{i=1}^n \lambda(d\dot{x}_i) \right. \\ &\quad \left. - \frac{1}{Z_R} \int_{\dot{\mathcal{M}}} \int_{\mathbb{R}^{dn}} \mathbb{1}_{\mathcal{D}}(\dot{\mathbf{x}}\dot{\mathbf{y}}) (F_A(\dot{\mathbf{x}}) \right. \\ &\quad \left. + \sum_{m=1}^{+\infty} \frac{z^m}{m!} \int_{B(0,R)^m} F_A(\dot{\mathbf{x}}\dot{x}_1 \dots \dot{x}_m) \prod_{k=1}^m \mathbb{1}_{\dot{x}_k \notin \mathbb{B}(\dot{\mathbf{x}})} \otimes_{k=1}^m d\dot{x}_k) \otimes_{i=1}^n \lambda(d\dot{x}_i) \pi|_{R^c}(d\dot{\mathbf{y}}) \right| \\ &\leq \int_{\dot{\mathcal{M}}} \left| \int_{\mathbb{R}^{dn}} F_A(\dot{\mathbf{x}}) \left(\frac{\mathbb{1}_{\mathcal{D}}(\dot{\mathbf{x}})}{Z_R} - \frac{\mathbb{1}_{\mathcal{D}}(\dot{\mathbf{x}}\dot{\mathbf{y}})}{Z_R} \right) \right. \\ &\quad \left. + \sum_{m=1}^{+\infty} \frac{z^m}{m!} \int_{\mathbb{R}^{dm}} F_A(\dot{\mathbf{x}}\dot{\mathbf{x}}) \prod_{k=1}^m (\mathbb{1}_{\dot{x}_k \notin \mathbb{B}(\dot{\mathbf{x}})} e^{-\psi^R(\dot{x}_k)} \right. \\ &\quad \left. \left(\frac{\mathbb{1}_{\mathcal{D}}(\dot{\mathbf{x}})}{Z_R} - \frac{\mathbb{1}_{\mathcal{D}}(\dot{\mathbf{x}}\dot{\mathbf{y}})}{Z_R} \mathbb{1}_{\mathbf{x} \subset B(0,R)} \right) \otimes_{k=1}^m d\dot{x}_k \otimes_{i=1}^n \lambda(d\dot{x}_i) \right| \pi|_{R^c}(d\dot{\mathbf{y}}). \end{aligned}$$

We then have that

$$\mathbf{d}_{TV}(R) \leq \left| \frac{\mathcal{Z}_R}{Z_R} - 1 \right| + n \left(1 + \frac{\mathcal{Z}_R}{Z_R} \right) \frac{e^{\dot{z}|B(0,R)|}}{\mathcal{Z}_R} e^{\dot{z} \int_{B(0,R)^c} e^{-\dot{\psi}^R(x)} dx} \int_{B(0,R-\overset{\circ}{r})^c} e^{-\dot{\psi}(x)} dx + \dot{z} \frac{\mathcal{Z}_R}{Z_R} \int_{B(0,R)^c} e^{-\dot{\psi}^R(x)} dx,$$

where the last inequality follows from the fact that the function F_A is bounded by one, and by carefully reordering and upperbounding each term.

We now need the following fine estimate on the asymptotic behaviour for large R of the two normalisation constants \mathcal{Z}_R and Z_R :

$$1 \leq \frac{\mathcal{Z}_R}{Z_R} \leq \exp \left(\dot{z} \int_{B(0,R)^c} e^{-\dot{\psi}^R(x)} dx \right),$$

where the upper bound tends fast to 1, since the exponent is summable in R , as stated in (2.2). Therefore, there exists a positive constant \mathfrak{c}_3 depending only on $n, \dot{\psi}, \dot{z}$ such that, for R large enough,

$$\begin{aligned} \mathbf{d}_{TV}(R) &\leq \mathfrak{c}_3 \left(\int_{B(0,R-\overset{\circ}{r})^c} e^{-\dot{\psi}(x)} dx + \int_{B(0,R)^c} e^{-\dot{\psi}^R(x)} dx \right) \\ &\leq \mathfrak{c}_3 \left(\frac{\int_{\mathbb{R}^d} |x|^2 e^{-\dot{\psi}(x)} dx}{(R-\overset{\circ}{r})^2} + \int_{B(0,R)^c} e^{-\dot{\psi}^R(x)} dx \right). \end{aligned} \tag{2.12}$$

Thanks to assumptions (2.1) and (2.2) on $\dot{\psi}$ and $\dot{\psi}^R$, respectively, the right-hand side is summable.

The convergence of the series in (2.11) implies for every \hat{R} the summability (2.9), which in turn implies that Ω_x is μ -a.s. a set of full measure. This completes the proof of Proposition 2.5. \square

We are then only left with proving Lemma 2.6.

Proof of Lemma 2.6. According to $(\mathfrak{S}_{m,R})$, for any $i \in \{1, \dots, n\}$, the process

$$\begin{aligned} \overset{\circ}{W}_i(t) &= \overset{\circ}{X}_i^{m,R}(t) - \overset{\circ}{X}_i^{m,R}(0) + \frac{1}{2} \int_0^t \nabla \dot{\psi}(\overset{\circ}{X}_i^{m,R}(s)) ds \\ &\quad - \sum_{j=1}^n \int_0^t (\overset{\circ}{X}_i^{m,R} - \overset{\circ}{X}_j^{m,R})(s) dL_{ij}(s) - \sum_{k'=1}^m \int_0^t (\overset{\circ}{X}_i^{m,R} - \overset{\circ}{X}_{k'}^{m,R})(s) d\ell_{ik'}(s) \end{aligned} \tag{2.13}$$

is a Brownian motion. Since $X^{m,R}$ is time-reversible, the process $\left(\overset{\circ}{X}_i^{m,R}(t) \right)_{t \in [0,1]}$ has the same distribution as the backward process $\left(\overset{\circ}{X}_i^{m,R}(1-t) \right)_{t \in [0,1]}$. Consequently the process $\overset{\circ}{\leftarrow} W_i$ obtained by replacing $\overset{\circ}{X}_i^{m,R}(\cdot)$ by $\overset{\circ}{X}_i^{m,R}(1-\cdot)$ in (2.13) is also a Brownian motion. Therefore, one can express $\overset{\circ}{X}_i^{m,R}(\cdot)$ – without local-time terms – as follows:

$$\overset{\circ}{X}_i^{m,R}(t) = \overset{\circ}{X}_i^{m,R}(0) + \frac{1}{2} (\overset{\circ}{W}_i(t) + \overset{\circ}{\leftarrow} W_i(1-t) - \overset{\circ}{\leftarrow} W_i(1)), \quad t \in [0, 1]. \tag{2.14}$$

Similarly,

$$\overset{\circ}{X}_k^{m,R}(t) = \overset{\circ}{X}_k^{m,R}(0) + \frac{1}{2} (\overset{\circ}{\dot{W}}_k(t) + \overset{\circ}{\dot{\leftarrow} W}_k(1-t) - \overset{\circ}{\dot{\leftarrow} W}_k(1)), \quad t \in [0, 1].$$

The $n + m$ components of $X^{m,R}$ are exchangeable, thus

$$P_{\bar{\nu}^{m,R}} \left(\exists i \leq n, \dot{X}_i^{m,R} \in \mathcal{B}(\alpha, \delta, \varepsilon) \text{ or } \exists k \leq m, \dot{X}_k^{m,R} \in \mathcal{B}(\alpha', \delta, \varepsilon) \right) \leq n P_{\bar{\nu}^{m,R}} \left(\dot{X}_1^{m,R} \in \mathcal{B}(\alpha, \delta, \varepsilon) \right) + m P_{\bar{\nu}^{m,R}} \left(\dot{X}_1^{m,R} \in \mathcal{B}(\alpha', \delta, \varepsilon) \right).$$

Summing over all possible initial positions, we get

$$P_{\bar{\nu}^{m,R}} \left(\dot{X}_1^{m,R} \in \mathcal{B}(\alpha, \delta, \varepsilon) \right) = \sum_{k=0}^{+\infty} P_{\bar{\nu}^{m,R}} \left(k\alpha \leq |\dot{X}_1^{m,R}(0)| < (k+1)\alpha \text{ and } \inf_{[0;1]} |\dot{X}_1^{m,R}| \leq \alpha \text{ and } w(\dot{X}_1^{m,R}, \delta) > \varepsilon \right).$$

A path which starts outside $B(0, k\alpha)$ and visits $B(0, \alpha)$ before time 1 has necessarily an oscillation larger than $(k - 1)\alpha\delta$ during some time interval of length δ ; moreover, for k large enough, $(k - 1)\alpha\delta$ is larger than ε . Therefore, the two first conditions in the above event imply the third one as soon as $k > 1 + \frac{\varepsilon}{\alpha\delta}$. Hence

$$P_{\bar{\nu}^{m,R}} \left(\dot{X}_1^{m,R} \in \mathcal{B}(\alpha, \delta, \varepsilon) \right) \leq P_{\bar{\nu}^{m,R}} \left(|\dot{X}_1^{m,R}(0)| < \alpha + \varepsilon/\delta \text{ and } w(\dot{X}_1^{m,R}, \delta) > \varepsilon \right) + \sum_{k > 1 + \varepsilon/\alpha\delta} P_{\bar{\nu}^{m,R}} \left(k\alpha \leq |\dot{X}_1^{m,R}(0)| < (k+1)\alpha \text{ and } w(\dot{X}_1^{m,R}, \delta) > (k-1)\alpha\delta \right).$$

Thanks to the decomposition (2.14),

$$w(\dot{X}_1^{m,R}, \delta) > \varepsilon \Rightarrow w(\dot{W}_1, \delta) > \varepsilon \text{ or } w(\dot{\underline{W}}_1, \delta) > \varepsilon.$$

Therefore, we have

$$P_{\bar{\nu}^{m,R}} \left(\dot{X}_1^{m,R} \in \mathcal{B}(\alpha, \delta, \varepsilon) \right) \leq P_{\bar{\nu}^{m,R}} \left(|\dot{X}_1^{m,R}(0)| < \alpha + \frac{\varepsilon}{\delta} \right) \left(P_{\bar{\nu}^{m,R}} \left(w(\dot{W}_1, \delta) > \varepsilon \right) + P_{\bar{\nu}^{m,R}} \left(w(\dot{\underline{W}}_1, \delta) > \varepsilon \right) \right) + \sum_{k > 1 + \varepsilon/\alpha\delta} \left(P_{\bar{\nu}^{m,R}} \left(w(\dot{W}_1, \delta) > (k-1)\alpha\delta \right) + P_{\bar{\nu}^{m,R}} \left(w(\dot{\underline{W}}_1, \delta) > (k-1)\alpha\delta \right) \right).$$

Note now the following standard estimate on the modulus of continuity of any d -dimensional Brownian motion W : there exist two universal constants $\mathfrak{c}_1 > 0$ and $\mathfrak{c}_2 > 0$, depending only on the dimension d , such that

$$P(w(W, \delta) \geq \varepsilon) \leq \frac{\mathfrak{c}_1}{4\delta} \exp\left(-\frac{\mathfrak{c}_2\varepsilon^2}{\delta}\right).$$

We then have

$$P_{\bar{\nu}^{m,R}} \left(\dot{X}_1^{m,R} \in \mathcal{B}(\alpha, \delta, \varepsilon) \right) \leq \frac{\mathfrak{c}_1}{2\delta} P_{\bar{\nu}^{m,R}} \left(|\dot{X}_1^{m,R}(0)| < \alpha + \frac{\varepsilon}{\delta} \right) \exp\left(-\frac{\mathfrak{c}_2\varepsilon^2}{\delta}\right) + \frac{\mathfrak{c}_1}{2\delta} \sum_{k > 1 + \varepsilon/\alpha\delta} \exp\left(-\mathfrak{c}_2(k-1)^2\alpha^2\delta\right) \leq \frac{\mathfrak{c}_1}{2\delta} \left(P_{\bar{\nu}^{m,R}} \left(|\dot{X}_1^{m,R}(0)| < \alpha + \frac{\varepsilon}{\delta} \right) + \sum_{j=0}^{+\infty} \exp\left(-\mathfrak{c}_2j\alpha^2\delta\right) \right) \exp\left(-\frac{\mathfrak{c}_2\varepsilon^2}{\delta}\right) \leq \frac{\mathfrak{c}_1}{\delta} \frac{1}{1 - \exp\left(-\mathfrak{c}_2\alpha^2\delta\right)} \exp\left(-\frac{\mathfrak{c}_2\varepsilon^2}{\delta}\right),$$

By similar arguments, we obtain the following upper bound for the particles:

$$P_{\bar{\nu}^{m,R}} \left(\dot{X}_1^{m,R} \in \mathcal{B}(\alpha', \delta, \varepsilon) \right) \leq \frac{\mathfrak{c}_1}{\delta} \frac{1}{1 - \exp(-\mathfrak{c}_2(\alpha')^2 \delta / \dot{\sigma}^2)} \exp\left(-\frac{\mathfrak{c}_2 \varepsilon^2}{\dot{\sigma}^2 \delta}\right).$$

Choosing $\mathfrak{c}_0 := \frac{\mathfrak{c}_2}{\max(1, \dot{\sigma}^2)}$ yields the claimed estimate. \square

2.2 A (two-type) equilibrium measure

The identification of equilibrium – versus reversible – measures associated to the dynamics (\mathfrak{S}) is mathematically and physically relevant. We address it in this section.

Proposition 2.8. Consider the solution of the two-type infinite-dimensional equation (\mathfrak{S}) , whose initial condition $X(0)$ is random and distributed according to the probability measure μ defined on \mathcal{M} by (2.8). This solution is time-reversible.

Proof. Recall that, thanks to Propositions 2.4 and 2.5, for any fixed admissible initial condition $\mathbf{x} \in \mathcal{D}$, we can construct a path $X^{\mathbf{x}}$ solving (\mathfrak{S}) on the full set $\Omega_{\mathbf{x}}$.

We aim to prove that the process X^{X_0} is time-reversible as soon as X_0 is a μ -distributed point process independent of the Brownian motions $(\dot{W}_i)_i$'s and $(\dot{W}_k)_k$'s.

The process X^{X_0} is time-reversible on $[0, 1]$ if, for any time T in $[0, 1]$, the backward process $(X^{X_0}(T - t))_{0 \leq t \leq T}$ has the same distribution as the forward process $(X^{X_0}(t))_{0 \leq t \leq T}$. Equivalently, one has to prove that, for any times $0 \leq t_1 < \dots < t_j \leq T$, $j \in \mathbb{N}$ and any bounded continuous local functions F_1, \dots, F_j on \mathcal{M} ,

$$\int_{\mathcal{D}} E \left(\prod_{i=1}^j F_i(X^{\mathbf{x}}(T - t_i)) - \prod_{i=1}^j F_i(X^{\mathbf{x}}(t_i)) \right) \mu(d\mathbf{x}) = 0.$$

Since $X^{\mathbf{x}}$ was obtained in Proposition 2.4 as limit of $(X^{\mathbf{x},R})_R$, it is sufficient to prove that

$$\lim_{R \rightarrow +\infty} \int_{\mathcal{D}} E \left(\prod_{i=1}^j F_i(X^{\mathbf{x},R}(T - t_i)) - \prod_{i=1}^j F_i(X^{\mathbf{x},R}(t_i)) \right) \mu(d\mathbf{x}) = 0.$$

In the same way as it was done in the proof of the existence of the two-type process, we split the computation of the integral term into two terms, introducing μ^R – see (2.10) – defined as a mixture of the measures $\nu^{m,R}$, themselves reversible under the finite dimensional dynamics $(\mathfrak{S}_{m,R})$. Therefore,

$$\begin{aligned} & \int_{\mathcal{D}} E \left(\prod_{i=1}^j F_i(X^{\mathbf{x},R}(T - t_i)) - \prod_{i=1}^j F_i(X^{\mathbf{x},R}(t_i)) \right) \mu(d\mathbf{x}) \\ & \leq \underbrace{\int_{\mathcal{D}} E \left(\prod_{i=1}^j F_i(X^{m(\mathbf{x},R),R}(T - t_i)) - \prod_{i=1}^j F_i(X^{m(\mathbf{x},R),R}(t_i)) \right) \mu^R(d\mathbf{x})}_{\text{vanishes due to reversibility}} + \prod_{i=1}^j \|F_i\|_{\infty} \mathbf{d}_{TV}(R) \end{aligned}$$

We proved in (2.12) the summability in R of the distance in total variation $\mathbf{d}_{TV}(R)$, thus a fortiori it tends to zero. This completes the proof of the time-reversibility of the solution of (\mathfrak{S}) when the initial condition is μ -distributed. \square

3 Occurrence of a new depletion interaction between hard spheres

We are interested now in the projection of the two-type infinite point process considered till now onto the system of just the n hard spheres. Our attention will first focus on the projection $\dot{\mu}$ of the reversible measure μ studied in Section 2.2. An new interaction between the hard spheres induced by the small ones will be observed as a *depletion interaction*. Its specific properties are pointed out, in particular the fact that it is highly local, see Figure 4 and Figure 5. We then identify an n -dimensional random gradient dynamics whose reversible measure is proportional to $\dot{\mu}$. Finally, we prove that, asymptotically as the density \dot{z} of the (hidden) particles tends to infinity, the measure $\dot{\mu}$ concentrates around remarkable geometrical configurations: they form sphere clusters that maximise their contact numbers, which is part of an important – and difficult – topic in discrete geometry.

3.1 The projection of the two-type equilibrium measure: The occurrence of a depletion interaction

We study here the projection of the equilibrium measure μ onto the n hard spheres.

We first mention that in the case $n = +\infty$, S. Jansen and D. Tsagkarogiannis computed in [13, 14] the projection of the *partition function* of a two-type grand canonical Gibbs process on the *infinite* system of hard spheres. They prove the emergence of an additional induced interaction between the spheres, identified as a *depletion* interaction. This kind of interaction was already known and studied in the physical literature, see, e.g., [19] and [17]. In our setting, however, where the number of hard spheres is finite – fixed to n –, this approach does not work anymore, in particular because the density of the hard spheres vanishes.

Recall that in Section 1.2 we defined a slightly enlarged version of the hard spheres \dot{x}_i by placing around them a spherical shell with size \dot{r} , called depletion shell. The new feature is that these enlarged spheres with radius $\overset{\circ}{r} = \dot{r} + \dot{r}$ may pairwise overlap, which will be at the origin of the depletion interaction.

Proposition 3.1. Consider μ , the equilibrium probability measure on \mathcal{M} of the two-type system defined by (2.8). Its projection onto the n hard sphere system is a probability measure $\dot{\mu}_z$ on $\dot{\mathcal{M}}$ defined as

$$\dot{\mu}_z(d\dot{\mathbf{x}}) = \frac{1}{Z_z} \exp(-\dot{z} \mathcal{E}(\dot{\mathbf{x}})) \mathbb{1}_{\mathcal{D}}(\dot{\mathbf{x}}) \otimes_{i=1}^n \lambda(d\dot{x}_i), \quad (3.1)$$

where $\mathcal{E}(\dot{\mathbf{x}})$, the energy of the configuration $\dot{\mathbf{x}} \in \dot{\mathcal{M}}$, is given by

$$\mathcal{E}(\dot{\mathbf{x}}) := \text{Vol}(\mathbb{B}(\dot{\mathbf{x}})) = \text{Vol}\left(\bigcup_{i=1}^n B(\dot{x}_i, \overset{\circ}{r})\right).$$

Proof. Integrating the measure μ over bounded test functions F supported on $\dot{\mathcal{M}}$ yields

$$\begin{aligned} \int_{\dot{\mathcal{M}}} F(\dot{\mathbf{x}}) \dot{\mu}_z(d\dot{\mathbf{x}}) &:= \int_{\mathcal{M}} F(\dot{\mathbf{x}}) \mu(d\mathbf{x}) = \frac{1}{Z_z} \int_{\mathbb{R}^{dn}} F(\dot{\mathbf{x}}) \int_{\dot{\mathcal{M}}} \mathbb{1}_{\mathcal{D}}(\dot{\mathbf{x}}\dot{\mathbf{x}}) \pi(d\dot{\mathbf{x}}) \otimes_{i=1}^n \lambda(d\dot{x}_i) \\ &= \frac{1}{Z_z} \int_{\mathbb{R}^{dn}} F(\dot{\mathbf{x}}) \left(\int_{\dot{\mathcal{M}}} \mathbb{1}_{\mathcal{D}}(\dot{\mathbf{x}}\dot{\mathbf{x}}|_{R(\dot{\mathbf{x}})}) \pi_{|R(\dot{\mathbf{x}})}(d\dot{\mathbf{x}}) \otimes \pi_{|R(\dot{\mathbf{x}})^c}(d\dot{\mathbf{x}}) \right) \mathbb{1}_{\mathcal{D}}(\dot{\mathbf{x}}) \otimes_{i=1}^n \lambda(d\dot{x}_i), \end{aligned}$$

where $R(\mathring{\mathbf{x}})$ is a radius large enough for $B(0, R(\mathring{\mathbf{x}}))$ to contain $\mathbb{B}(\mathring{\mathbf{x}})$. Since the particles outside of $B(0, R(\mathring{\mathbf{x}}))$ are independent of the ones inside, we get

$$\begin{aligned} \int_{\mathcal{M}} F(\mathring{\mathbf{x}}) \dot{\mu}_z(d\mathring{\mathbf{x}}) &= \frac{1}{Z_z} \int_{\mathbb{R}^{dn}} F(\mathring{\mathbf{x}}) \int_{\mathcal{M}} \mathbf{1}_{\mathbb{B}(\mathring{\mathbf{x}})^c}(\dot{\mathbf{x}}) \pi_{|_{R(\mathring{\mathbf{x}})}}(d\dot{\mathbf{x}}) \mathbf{1}_{\mathcal{D}}(\mathring{\mathbf{x}}) \otimes_{i=1}^n \lambda(d\dot{x}_i) \\ &= \frac{1}{Z_z} \int_{\mathbb{R}^{dn}} F(\mathring{\mathbf{x}}) \exp(-z \text{Vol}(\mathbb{B}(\mathring{\mathbf{x}}))) \mathbf{1}_{\mathcal{D}}(\mathring{\mathbf{x}}) \otimes_{i=1}^n \lambda(d\dot{x}_i), \end{aligned}$$

which is equivalent to the claim. \square

Remark 3.2. By the inclusion-exclusion rule,

$$\mathcal{E}(\mathring{\mathbf{x}}) = \sum_{k=1}^n \text{Vol}\left(B(\mathring{x}_k, \mathring{r})\right) + \sum_{k=2}^n \sum_{1 \leq i_1 < \dots < i_k \leq n} \varphi_k(\mathring{x}_{i_1}, \dots, \mathring{x}_{i_k}), \quad (3.2)$$

where the function φ_k , $k \geq 2$, is a symmetric translation-invariant function on $(\mathbb{R}^d)^k$ given by

$$\varphi_k(x_1, \dots, x_k) := (-1)^{k-1} \text{Vol}\left(B(x_1, \mathring{r}) \cap \dots \cap B(x_k, \mathring{r})\right). \quad (3.3)$$

The function φ_k is called the k -body *depletion interaction*. It is highly dependent on ρ , the proportionality factor between the particle radius and the hard sphere radius.

Putting it together yields

$$\dot{\mu}_z(d\mathring{\mathbf{x}}) = \exp\left(-z \left(nv_d \mathring{r}^d + \sum_{k=2}^n \sum_{1 \leq i_1 < \dots < i_k \leq n} \varphi_k(\mathring{x}_{i_1}, \dots, \mathring{x}_{i_k})\right)\right) \mathbf{1}_{\mathcal{D}}(\mathring{\mathbf{x}}) \otimes_{i=1}^n \lambda(d\dot{x}_i),$$

where v_d denotes the volume in \mathbb{R}^d of the unit sphere.

In the following lemma, we find thresholds on ρ , the ratio of particle and hard-sphere radii, in order for three-body or k -body interactions occur. See also [26] for a geometric computation in the case of differently shaped bodies.

Lemma 3.3. The multi-body depletion interaction reduces to a pair interaction as soon as the size proportionality factor ρ between the particles and the hard spheres is bounded from above by $\rho_2 := \frac{2}{3}\sqrt{3} - 1 \simeq 0.1547$. Moreover, 4-body depletion interactions can appear, in dimension $d = 2$, only if $\rho > \rho_3 := \sqrt{2} - 1 \simeq 0.4142$, in dimension $d \geq 3$, only if $\rho > \rho_3 := \sqrt{3/2} - 1 \simeq 0.2247$.

Proof. We first show that for $\rho \leq \rho_2$, the k -body interaction φ_k vanishes for any $k \geq 3$. Indeed, in any dimension $d \geq 2$, the lowest value of ρ for multiple depletion shells to overlap can be computed by considering 3 spheres whose centres lie on the vertices of an equilateral triangle of side-length $2\mathring{r}$, see the top of Figure 2.

There is overlap as soon as the centre of the triangle is at a distance $\mathring{r} = \mathring{r}(1 + \rho)$ from the vertices, that is if and only if

$$2\mathring{r} \frac{\sqrt{3}}{3} < \mathring{r} \iff 2 \frac{\sqrt{3}}{3} < 1 + \rho \iff \rho > \rho_2 := \frac{2}{3}\sqrt{3} - 1 \simeq 0.1547.$$

The value for ρ_3 depends on the dimension d . In dimension $d = 2$, the smallest value of ρ for more than 3 depletion shells to overlap is obtained by considering 4 spheres whose centres lie on the

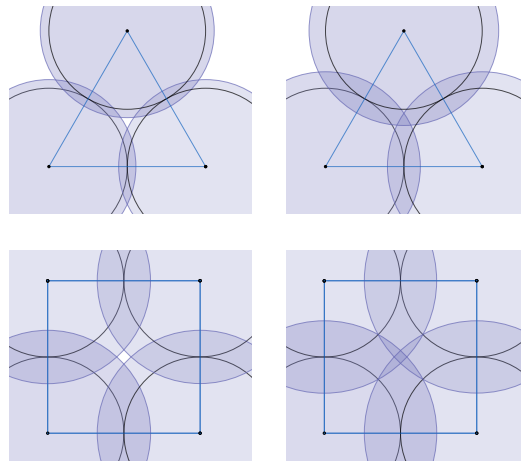


Figure 2: Examples of hard discs with depletion shell; the shaded areas represent the overlap between the depletion shells.

Top: In the picture on the left, $\rho \leq \rho_2$, while in the one on the right, $\rho > \rho_2$.

Bottom: In the picture on the left, $\rho_2 < \rho < \rho_3$, while in the one on the right, $\rho > \rho_3$.

vertices of a square of side-length $2\overset{\circ}{r}$, see the bottom of Figure 2. So, there is a 4-way overlap if and only if

$$2\sqrt{2}\overset{\circ}{r} < 2\overset{\circ}{r} \iff \rho > \rho_3 := \sqrt{2} - 1 \simeq 0.4142.$$

In dimension $d \geq 3$, the smallest value of ρ is obtained by considering 4 spheres whose centres lie on the vertices of a regular tetrahedron of side-length $2\overset{\circ}{r}$. So, there is a 4-way overlap if and only if the distance between any vertex and the center of mass of the tetrahedron is smaller than $\overset{\circ}{r}$, that is

$$\sqrt{3/2}\overset{\circ}{r} < \overset{\circ}{r} \iff \rho > \rho_3 := \sqrt{3/2} - 1 \simeq 0.2247.$$

This concludes the proof. □

Let us compute the pair depletion interaction φ_2 in any dimension.

Lemma 3.4. The pair depletion interaction is attractive, radial and strongly local. Its expression in dimension d is given by the following integral: for any $x_i, x_j \in \mathbb{R}^d$,

$$\varphi_2(x_i, x_j) = -2v_{d-1}\overset{\circ}{r}^d \int_0^{\arccos(u)} (\sin \theta)^d d\theta \mathbb{1}_{[\frac{1}{1+\rho}, 1]}(u), \text{ where } u := \frac{|x_i - x_j|}{2\overset{\circ}{r}}.$$

Proof. Note first that the function $\varphi_2(x_i, x_j) = -\text{Vol} \left(B(x_i, \overset{\circ}{r}) \cap B(x_j, \overset{\circ}{r}) \right)$ is non-positive and therefore the pair depletion interaction is attractive.

Moreover, it only depends on the distance between both points x_i and x_j in \mathbb{R}^d . Therefore, to simplify the notations we define the (rescaled) function $\mathcal{V}_{\text{ovlap}}$ as follows:

$$\mathcal{V}_{\text{ovlap}}(u) := -\varphi_2(x_i, x_j) \text{ with } u = \frac{|x_i - x_j|}{2\overset{\circ}{r}} \in \left[\frac{\overset{\circ}{r}}{\overset{\circ}{r}}, +\infty \right). \tag{3.4}$$

The function $\mathcal{V}_{\text{ovlap}}$ is clearly decreasing from its maximal value $\mathcal{V}_{\text{ovlap}}^*$ – attained at $u = \frac{\overset{\circ}{r}}{\overset{\circ}{r}} = \frac{1}{1+\rho}$ – to its minimal value 0 attained at $u = 1$. It vanishes on $[1, +\infty)$, underlining the strong locality of this pair interaction. We compute it now.

By shift invariance and symmetry, denoting (e_1, \dots, e_d) an orthonormal basis of \mathbb{R}^d , we find

$$\begin{aligned} \mathcal{V}_{\text{ovlap}}(u) &= \text{Vol} \left(B(0, \overset{\circ}{r}) \cap B(2\overset{\circ}{r}u e_1, \overset{\circ}{r}) \right) \\ &= 2 \text{Vol} \left(\left\{ x \in \mathbb{R}^d, |x| \leq \overset{\circ}{r} \text{ and } x \cdot e_1 \geq \overset{\circ}{r}u \right\} \right) \\ &= 2 \text{Vol} \left(\left\{ x \in \mathbb{R}^d, \sum_{i=2}^d (x \cdot e_i)^2 \leq \overset{\circ}{r}^2 - (x \cdot e_1)^2 \text{ and } x \cdot e_1 \geq \overset{\circ}{r}u \right\} \right). \end{aligned}$$

Introducing v_{d-1} , the volume of the unit sphere in \mathbb{R}^{d-1} , one gets for $\frac{1}{1+\rho} \leq u \leq 1$,

$$\begin{aligned} \mathcal{V}_{\text{ovlap}}(u) &= 2 \int_{\overset{\circ}{r}u}^{\overset{\circ}{r}} v_{d-1} \left(\sqrt{\overset{\circ}{r}^2 - t^2} \right)^{d-1} dt = 2v_{d-1} (\overset{\circ}{r}^2)^{\frac{d-1}{2}} \int_u^1 \left(\sqrt{1 - s^2} \right)^{d-1} \overset{\circ}{r} ds \\ &= 2v_{d-1} \overset{\circ}{r}^d \int_0^{\arccos(u)} (\sin \theta)^d d\theta. \end{aligned} \quad \square$$

Example 3.5 (The pair depletion interaction between discs in \mathbb{R}^2).

Experimental results in \mathbb{R}^2 were obtained by physicists to estimate the value of the depletion potential, see, e.g., [20, Figure 3].

Applying Lemma 3.4 one can compute explicitly the integral in the case $d = 2$ to obtain, for $u = \frac{|x_i - x_j|}{2\overset{\circ}{r}} \in [\frac{1}{1+\rho}, 1]$,

$$\varphi_2(x_i, x_j) = -2 v_1 \overset{\circ}{r}^2 \int_0^{\arccos(u)} (\sin \theta)^2 d\theta = -2\overset{\circ}{r}^2 \left(\arccos(u) - u\sqrt{1 - u^2} \right).$$

It can also be computed directly via the following simple planar geometry argument (cf. Figure 3).

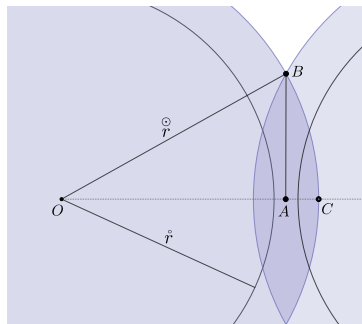


Figure 3: Intersection of two depletion discs.

In the plane, consider a disc centred at a point $O \in \mathbb{R}^2$, with radius $\overset{\circ}{r}$, and suppose it intersects another disc of the same radius and whose centre is at distance $2\overset{\circ}{r}u$ from O .

Denote by $\mathcal{A}_{\text{sec}}(u)$, the area of the circular sector in OBC . Consider then the area $\mathcal{A}_{\text{tri}}(u)$ of the rectangular triangle OBC . One has

$$\mathcal{A}_{\text{sec}}(u) = \frac{1}{2} \arccos(u) \overset{\circ}{r}^2, \quad \mathcal{A}_{\text{tri}}(u) = \frac{1}{2} \overline{OA} \overline{AB} = \frac{\overset{\circ}{r}^2}{2} u\sqrt{1 - u^2}.$$

The area of the overlap is then given by

$$\mathcal{V}_{\text{ovlap}}(u) = 4(\mathcal{A}_{\text{sec}}(u) - \mathcal{A}_{\text{tri}}(u)) = 2\overset{\circ}{r}^2 \left(\arccos(u) - u\sqrt{1 - u^2} \right), \quad (3.5)$$

see Figure 4, left. The maximal overlap area is

$$\mathcal{V}_{\text{ovlap}}^* = \mathcal{V}_{\text{ovlap}}\left(\frac{1}{1+\rho}\right) = 2\overset{\circ}{r}{}^2 \left(\arccos\left(\frac{1}{1+\rho}\right) - \frac{1}{(1+\rho)^2} \sqrt{\rho(2+\rho)} \right). \quad (3.6)$$

Moreover, the derivative on $(\frac{1}{1+\rho}, 1)$ of the function $\mathcal{V}_{\text{ovlap}}$ is given by

$$\mathcal{V}'_{\text{ovlap}}(u) = -4\overset{\circ}{r}{}^2 \sqrt{1-u^2}$$

which vanishes in 1 (see Figure 4, right). Therefore the function $\mathcal{V}_{\text{ovlap}}$ is of class C^1 over the full interval $[\frac{1}{1+\rho}, +\infty)$. Nevertheless its second derivative explodes at the point $u = 1$ since

$$\mathcal{V}''_{\text{ovlap}}(u) = 4\overset{\circ}{r}{}^2 \frac{u}{\sqrt{1-u^2}}, \quad \frac{1}{1+\rho} \leq u < 1.$$

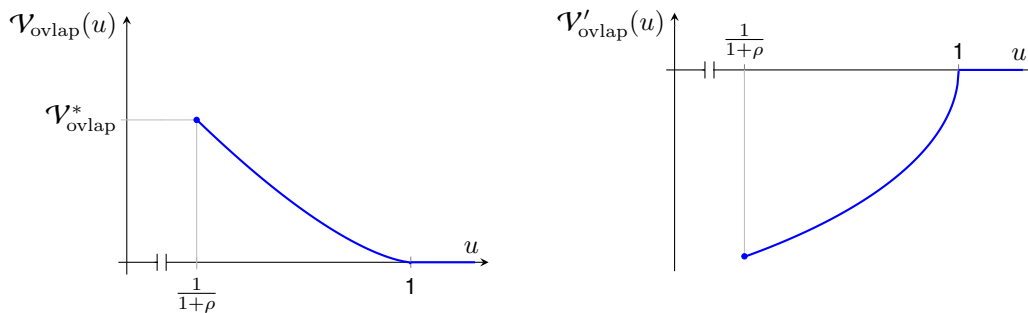


Figure 4: Behaviour of $u \mapsto \mathcal{V}_{\text{ovlap}}(u)$ (left) and $u \mapsto \mathcal{V}'_{\text{ovlap}}(u)$ (right) for discs in the plane.

Remark 3.6. If the size of the particles is large enough ($\rho > \rho_2$), then a three-body depletion interaction can appear. Its explicit computation is done in [15, Equation 2.2]:

$$\begin{aligned} \varphi_3(x_1, x_2, x_3) &= \frac{1}{2} \left(\sum_{\{i,j\} \subset \{1,2,3\}} \mathcal{V}_{\text{ovlap}}\left(\frac{|x_i - x_j|}{2\overset{\circ}{r}}\right) - \pi\overset{\circ}{r}{}^2 \right. \\ &\quad \left. + \frac{1}{2} \sqrt{4|x_1 - x_2|^2|x_1 - x_3|^2 - (|x_1 - x_2|^2 + |x_1 - x_3|^2 - |x_2 - x_3|^2)^2} \right). \end{aligned}$$

Example 3.7 (The pair depletion interaction between balls in \mathbb{R}^3).

In the 3-dimensional Euclidean space, experimental results for the value of the depletion interaction are obtained, e.g., as in [20, Figure 5].

Applying Lemma 3.4 in the case $d = 3$, one can explicitly compute the integral and obtain, for $u \in [\frac{1}{1+\rho}, 1]$:

$$\mathcal{V}_{\text{ovlap}}(u) = 2v_2\overset{\circ}{r}{}^3 \int_0^{\arccos(u)} (\sin \theta)^3 d\theta = 2\pi\overset{\circ}{r}{}^3 \int_u^1 (1-s^2) ds = \frac{4\pi}{3}\overset{\circ}{r}{}^3 (1-u)^2 \left(1 + \frac{u}{2}\right),$$

see also, e.g., [25]. Its maximal value is given by

$$\mathcal{V}_{\text{ovlap}}^* = \mathcal{V}_{\text{ovlap}}\left(\frac{1}{1+\rho}\right) = 2\pi\overset{\circ}{r}{}^3 \rho^2 \left(1 + \frac{2}{3}\rho\right). \quad (3.7)$$

Its first derivative satisfies

$$\mathcal{V}'_{\text{ovlap}}(u) = -2\pi \overset{\circ}{r}{}^3(1-u^2), \quad \frac{1}{1+\rho} < u < 1.$$

This expression vanishes in 1 which implies – as in dimension 2 – the C^1 -regularity of the function $\mathcal{V}_{\text{ovlap}}$ over the full interval $[\frac{1}{1+\rho}, +\infty)$, see Figure 5, left. Its second derivative on $(\frac{1}{1+\rho}, 1)$ satisfies $\mathcal{V}''_{\text{ovlap}}(u) = 4\pi \overset{\circ}{r}{}^3 u$ which does not vanish at $u = 1$ but remains bounded, contrary to the behaviour in dimension 2, see Figure 5, right.

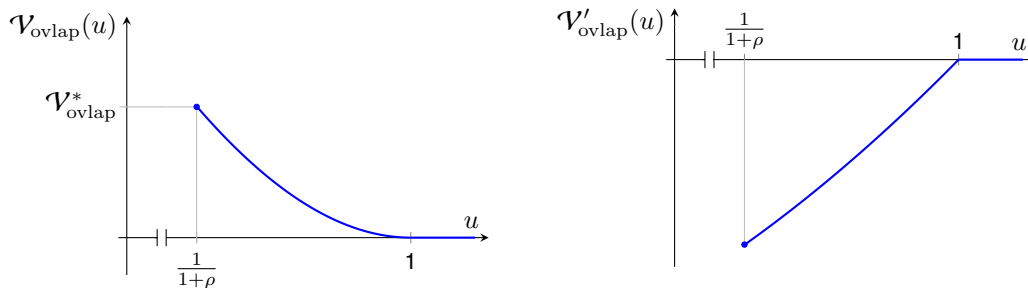


Figure 5: Behaviour of $u \mapsto \mathcal{V}_{\text{ovlap}}(u)$ (left) and $u \mapsto \mathcal{V}'_{\text{ovlap}}(u)$ (right) for balls in \mathbb{R}^3 .

Notice that, if the size of the particles is large enough ($\rho > \rho_2$), then a three-body depletion interaction can appear. K. W. Kratky computes it implicitly in [16, Equation 1.2b].

3.2 An associated gradient dynamics

From now on, we suppose $\rho \leq \rho_2$, so that the energy of a configuration of hard spheres defined by (3.2) is only generated by pairwise interactions. Due to Lemma 3.4 and the definition of the overlap function (3.4), the energy function becomes

$$\mathcal{E}(\overset{\circ}{\mathbf{x}}) = nv_d \overset{\circ}{r}{}^d - \sum_{1 \leq i < j \leq n} \mathcal{V}_{\text{ovlap}}\left(\frac{|\overset{\circ}{x}_i - \overset{\circ}{x}_j|}{2\overset{\circ}{r}}\right). \quad (3.8)$$

Therefore, using the explicit expression of $\mathcal{V}_{\text{ovlap}}$ and $\mathcal{V}'_{\text{ovlap}}$, the gradient field of the energy satisfies, for $i \in \{1, \dots, d\}$,

$$\begin{aligned} \nabla_i \mathcal{E}(\overset{\circ}{\mathbf{x}}) &= -\frac{1}{2\overset{\circ}{r}} \sum_{j=1}^n \mathcal{V}'_{\text{ovlap}}\left(\frac{|\overset{\circ}{x}_i - \overset{\circ}{x}_j|}{2\overset{\circ}{r}}\right) \frac{\overset{\circ}{x}_i - \overset{\circ}{x}_j}{|\overset{\circ}{x}_i - \overset{\circ}{x}_j|} \\ &= -v_{d-1} \overset{\circ}{r}{}^{d-1} \sum_{j=1}^n \left(1 - \frac{|\overset{\circ}{x}_i - \overset{\circ}{x}_j|^2}{4\overset{\circ}{r}{}^2}\right)_+^{\frac{d-1}{2}} \frac{\overset{\circ}{x}_i - \overset{\circ}{x}_j}{|\overset{\circ}{x}_i - \overset{\circ}{x}_j|}, \end{aligned} \quad (3.9)$$

where, as usual, $u_+ := \max(0, u)$ denotes the positive part of any real number u .

Let us now define the diffusive dynamics of the hard spheres $(\overset{\circ}{X}_i)_{i=1, \dots, n}$ submitted to (\dot{z} times) this

gradient field. It solves the SDE

$$\left\{ \begin{array}{l} \text{for } i \in \{1, \dots, n\}, t \in [0, 1], \\ d\dot{X}_i(t) = d\dot{W}_i(t) - \frac{1}{2} \nabla \psi(\dot{X}_i(t)) dt \\ \quad + \frac{\dot{z}}{2} v_{d-1} \overset{\circ}{r}^{d-1} \sum_{j=1}^n \left(1 - \frac{|\dot{X}_i - \dot{X}_j|^2}{4\overset{\circ}{r}^2} \right)_+ \frac{\dot{X}_i - \dot{X}_j}{|\dot{X}_i - \dot{X}_j|} dt \\ \quad + \sum_{j=1}^n (\dot{X}_i(t) - \dot{X}_j(t)) dL_{ij}(t), \\ L_{ij}(0) = 0, \quad L_{ij} \equiv L_{ji}, \quad L_{ij}(t) = \int_0^t \mathbb{1}_{|\dot{X}_i(s) - \dot{X}_j(s)| = 2\overset{\circ}{r}} dL_{ij}(s), \quad L_{ii} \equiv 0, \end{array} \right. \quad (\mathfrak{S}_n^{\text{dep}})$$

where $\dot{W}_1, \dots, \dot{W}_n$ are n independent \mathbb{R}^d -valued Brownian motions and L_{ij} denotes the collision local time between the sphere i and the sphere j . The local times L_{ij} describe the effects of the elastic collision between the large particles i and j (subject to normal reflection).

Theorem 3.8. The SDE $(\mathfrak{S}_n^{\text{dep}})$ admits a unique solution in the set of admissible configurations \mathcal{D} . Moreover the measure $\overset{\circ}{\mu}_z$ defined by (3.1) is reversible under this dynamics.

Proof. The stochastic differential system $(\mathfrak{S}_n^{\text{dep}})$ describes the dynamics of an nd -dimensional gradient diffusion with reflection at the boundary of the set of admissible hard spheres $\mathcal{D} \cap \overset{\circ}{\mathcal{M}} = \bigcap_{1 \leq i < j \leq n} \left\{ \overset{\circ}{\mathbf{x}} \in \overset{\circ}{\mathcal{M}} : \Gamma_{ij}(\overset{\circ}{\mathbf{x}}) \geq 0 \right\}$. This domain is induced by the pairwise constraint functions $\Gamma_{ij}(\overset{\circ}{\mathbf{x}}) := \frac{|\overset{\circ}{x}_i - \overset{\circ}{x}_j|^2}{4\overset{\circ}{r}^2} - 1$ introduced in (2.4).

We first verify the smoothness of each constraint function and their global compatibility: this was already done in steps (i) and (ii) of the proof of Proposition 2.2 for a larger number of constraints.

Existence and uniqueness of a strong solution to $(\mathfrak{S}_n^{\text{dep}})$ are then ensured by [9, Theorem 2.2] as soon as the gradient field of the energy function is Lipschitz continuous and bounded on the domain $\mathcal{D} \cap \overset{\circ}{\mathcal{M}}$. Considering the expression (3.9), this is the case in any dimension $d > 2$.

In dimension $d = 2$, however,

$$\nabla_i \mathcal{E}(\overset{\circ}{\mathbf{x}}) = -2\overset{\circ}{r} \sum_{j=1}^n \sqrt{\left(1 - \frac{|\overset{\circ}{x}_i - \overset{\circ}{x}_j|^2}{4\overset{\circ}{r}^2} \right)_+} \frac{\overset{\circ}{x}_i - \overset{\circ}{x}_j}{|\overset{\circ}{x}_i - \overset{\circ}{x}_j|}$$

is Lipschitz continuous on $\mathcal{D} \cap \overset{\circ}{\mathcal{M}}$ except around the configurations containing a pair of hard spheres whose centres lie at the critical distance $2\overset{\circ}{r} = 2\overset{\circ}{r}(1+\rho)$. This pathology corresponds to the explosion of the function $\mathcal{V}_{\text{ovlap}}''$ at $u = 1$ observed in Example 3.5. Nevertheless, the SDE $(\mathfrak{S}_n^{\text{dep}})$ can be solved straightforwardly as follows.

The solution is constructed progressively on intervals defined through a sequence of stopping times indicating, (i) either the moment in which a pair i, j of hard spheres is close enough, say $\Gamma_{ij}(\overset{\circ}{\mathbf{x}}) \in [0, \rho]$, or (ii) the moment in which two spheres are close to the critical distance, say $\Gamma_{ij}(\overset{\circ}{\mathbf{x}}) \in [2\rho, 2\rho(1 + \rho/2)]$. In the first kind of time interval, the energy function is smooth and we can use the existence result used for $d > 2$. In the second kind of time interval, the energy function is not smooth anymore, but the hard spheres cannot collide, meaning that $(\mathfrak{S}_n^{\text{dep}})$ does not contain collision local times. Therefore, we can apply strong existence results for Brownian diffusions with bounded Borel drift as, e.g., [24, Theorem 1].

Applying [9, Theorem 2.5] (see also [21]), we get that $\mathbb{1}_{\mathcal{D}}(\overset{\circ}{\mathbf{x}}) e^{-z\mathcal{E}(\overset{\circ}{\mathbf{x}})} d\overset{\circ}{\mathbf{x}}$ is a time-reversible measure for the dynamics $(\mathfrak{S}_{m,R})$. This concludes the proof of the theorem. \square

3.3 High-density of the small-particle bath: towards an optimal packing of finitely-many hard spheres

In Proposition 3.1, we saw that the log-density of the equilibrium measure $\hat{\mu}_z$ of the large spheres is proportional to the activity z of the bath of particles (i.e., the medium) in which they evolve. It is therefore natural to consider the asymptotic behaviour of the measure $\hat{\mu}_z$ in a high-density regime of the bath, that is for z tending to ∞ .

Heuristically, for a fixed activity z , the probability measure $\hat{\mu}_z$ favours the n -ball configurations with low energy. As z increases, $\hat{\mu}_z$ will concentrate more and more on configurations with minimal energy, as expressed in Proposition 3.9, below.

We further assume in this section that $\rho \leq \rho_2$.

The *contact number* $c_n(\hat{\mathbf{x}})$ of a configuration $\hat{\mathbf{x}} \in \mathcal{D}$ of n hard spheres is the number of its pair contacts:

$$c_n(\hat{\mathbf{x}}) := \#\{(i, j) \text{ s.t. } |\hat{x}_i - \hat{x}_j| = 2\hat{r}, 1 \leq i < j \leq n\}.$$

Proposition 3.9. Asymptotically in z , the equilibrium probability measure $\hat{\mu}_z$ of n hard spheres in \mathbb{R}^d that are submitted to the depletion force concentrates around cluster configurations which maximise the contact number of n spheres in \mathbb{R}^d .

More precisely, let $\mathcal{E}_* := \inf_{\hat{\mathbf{y}} \in \mathcal{D}} \mathcal{E}(\hat{\mathbf{y}})$ be the minimal energy of admissible hard-sphere configurations, and define the set of admissible configurations with η -minimal energy by $\mathcal{D}_*^\eta := \{\hat{\mathbf{y}} \in \mathcal{D}, \mathcal{E}(\hat{\mathbf{y}}) \leq \mathcal{E}_* + \eta\}$. Then

$$\forall \varepsilon, \eta > 0 \exists \hat{z}^* > 0, \forall z > \hat{z}^* \quad \hat{\mu}_z(\mathcal{D}_*^\eta) \geq 1 - \varepsilon. \quad (3.10)$$

Moreover, sphere configurations $\hat{\mathbf{x}} \in \mathcal{D}$ whose energy realises the minimum \mathcal{E}_* maximise the contact number $c(\hat{\mathbf{x}})$.

Proof. We first prove (3.10).

Since $Z_z := \int_{\mathcal{D}} e^{-z\mathcal{E}(\hat{\mathbf{x}})} \lambda^{\otimes n}(d\hat{\mathbf{x}})$ is a normalisation constant, one has

$$\begin{aligned} \hat{\mu}_z((\mathcal{D}_*^\eta)^c) &= \frac{\int_{\mathcal{D}} e^{-z\mathcal{E}(\hat{\mathbf{x}})} \mathbb{1}_{\mathcal{E}(\hat{\mathbf{x}}) > \mathcal{E}_* + \eta} \lambda^{\otimes n}(d\hat{\mathbf{x}})}{\int_{\mathcal{D}} e^{-z\mathcal{E}(\hat{\mathbf{x}})} \lambda^{\otimes n}(d\hat{\mathbf{x}})} = \frac{\int_{\mathcal{D}} e^{-z(\mathcal{E}(\hat{\mathbf{x}}) - (\mathcal{E}_* + \eta))} \mathbb{1}_{\mathcal{E}(\hat{\mathbf{x}}) > \mathcal{E}_* + \eta} \lambda^{\otimes n}(d\hat{\mathbf{x}})}{\int_{\mathcal{D}} e^{-z(\mathcal{E}(\hat{\mathbf{x}}) - (\mathcal{E}_* + \eta))} \lambda^{\otimes n}(d\hat{\mathbf{x}})} \\ &\leq \frac{\int_{\mathcal{D}} e^{-z(\mathcal{E}(\hat{\mathbf{x}}) - (\mathcal{E}_* + \eta))} \mathbb{1}_{\mathcal{E}(\hat{\mathbf{x}}) > \mathcal{E}_* + \eta} \lambda^{\otimes n}(d\hat{\mathbf{x}})}{\int_{\mathcal{D}} e^{-z(\mathcal{E}(\hat{\mathbf{x}}) - (\mathcal{E}_* + \eta))} \mathbb{1}_{\mathcal{E}(\hat{\mathbf{x}}) \leq \mathcal{E}_* + \eta} \lambda^{\otimes n}(d\hat{\mathbf{x}})} \\ &\leq \frac{\int_{\mathcal{D}} e^{-z(\mathcal{E}(\hat{\mathbf{x}}) - (\mathcal{E}_* + \eta))} \mathbb{1}_{\mathcal{E}(\hat{\mathbf{x}}) > \mathcal{E}_* + \eta} \lambda^{\otimes n}(d\hat{\mathbf{x}})}{\lambda^{\otimes n}(\{\hat{\mathbf{x}} \in \mathcal{D} : \mathcal{E}(\hat{\mathbf{x}}) \leq \mathcal{E}_* + \eta\})} =: \frac{\mathbf{n}(\eta, z)}{\mathbf{d}(\eta)}. \end{aligned}$$

Note that the denominator $\mathbf{d}(\eta)$ is positive and does not depend on z . For the numerator, note that for each fixed η , point-wise in $\hat{\mathbf{x}}$,

$$\lim_{z \nearrow \infty} e^{-z(\mathcal{E}(\hat{\mathbf{x}}) - (\mathcal{E}_* + \eta))} \mathbb{1}_{\mathcal{E}(\hat{\mathbf{x}}) > \mathcal{E}_* + \eta} = 0$$

Since $\hat{\mathbf{x}} \mapsto e^{-z(\mathcal{E}(\hat{\mathbf{x}}) - (\mathcal{E}_* + \eta))} \mathbb{1}_{\mathcal{E}(\hat{\mathbf{x}}) > \mathcal{E}_* + \eta}$ is uniformly bounded by the constant 1, which is $\lambda^{\otimes n}$ -integrable, the dominated convergence theorem implies that the numerator $\mathbf{n}(\eta, z)$ vanishes as z increases. This completes the proof of (3.10).

Next, we investigate the shape of the admissible configurations whose energy realises the minimum \mathcal{E}_* . Recalling (3.8),

$$\mathcal{E}(\dot{\mathbf{x}}) = nv_d \overset{\circ}{r}^d - \sum_{1 \leq i < j \leq n} \mathcal{V}_{\text{ovlap}}\left(\frac{|\dot{x}_i - \dot{x}_j|}{2\overset{\circ}{r}}\right).$$

Thus,

$$\begin{aligned} \mathcal{E}_* &= \inf_{\dot{\mathbf{x}} \in \mathcal{D}} \mathcal{E}(\dot{\mathbf{x}}) = nv_d \overset{\circ}{r}^d - \max_{\dot{\mathbf{x}} \in \mathcal{D}} \sum_{1 \leq i < j \leq n} \mathcal{V}_{\text{ovlap}}\left(\frac{|\dot{\mathbf{x}}_i - \dot{\mathbf{x}}_j|}{2\overset{\circ}{r}}\right) \\ &= nv_d \overset{\circ}{r}^d - c(n, d) \mathcal{V}_{\text{ovlap}}^*, \end{aligned} \tag{3.11}$$

where

$$c(n, d) := \max\{c_n(\dot{\mathbf{x}}), \dot{\mathbf{x}} = \{\dot{x}_1, \dots, \dot{x}_n\} \in \mathcal{D} \subset \mathbb{R}^d\}$$

is the maximum of the contact number of n non-overlapping identical spheres in \mathbb{R}^d . Thus the configurations $\dot{\mathbf{x}}$ that minimise the energy are maximising their contact number $c(\dot{\mathbf{x}})$, as claimed. \square

The identification of the set of configurations whose contact number equals $c(n, d)$ is a difficult topic, even in low dimensions 2 and 3, as it is presented in the next examples.

Recall that $c(n, d)$ is also the maximum number of edges that a contact graph of n non-overlapping translations of $B(0, 1)$ can have in \mathbb{R}^d , see, e.g., the monograph [3] and [4, Chapter 3]. Using this approach, we now review in more detail the situation in the Euclidean spaces \mathbb{R}^2 and \mathbb{R}^3 .

Example 3.10 (The planar case, $d = 2$). An explicit general formula for $c(n, 2)$ was introduced by Erdős in 1946, but rigorously established only in 1974 by Harborth, [11]:

$$c(n, 2) = \lfloor 3n - \sqrt{12n - 3} \rfloor, \quad n \geq 2.$$

In particular, one has

$$c(2, 2) = 1, \quad c(3, 2) = 3, \quad c(4, 2) = 5, \quad c(5, 2) = 7, \quad c(6, 2) = 9, \quad c(7, 2) = 12.$$

Moreover, the hexagonal packing arrangement is a cluster configuration whose contact number achieves $c(n, 2)$ for all n , see Figure 6. But it also corresponds to clusters which realise the densest packing. Nevertheless, the problem of recognising (all) contact graphs of unit disc packing is NP-hard, see [6].

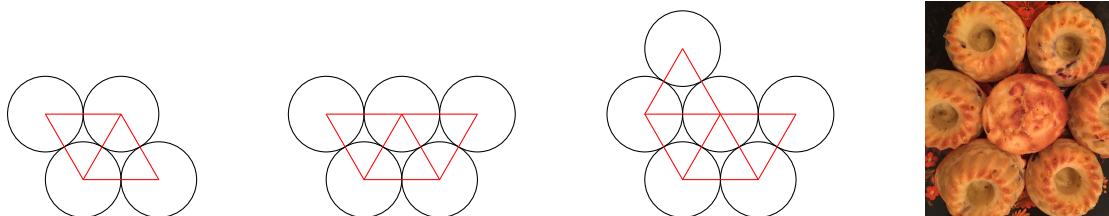


Figure 6: Favourite planar cluster configurations with minimal energy \mathcal{E}_* for $n = 4, 5, 6$ and their induced contact graphs with respectively $c(n, 2)$ contacts. Optimal Kugelhopf configuration for $n = 7$.

We now study the asymptotic behaviour of the minimal energy \mathcal{E}_* for small ρ . It means that we expand the maximal overlap area obtained in (3.6)

$$\mathcal{V}_{\text{ovlap}}^* = 2\overset{\circ}{r}^2 \left(\arccos\left(\frac{1}{1+\rho}\right) - \frac{1}{(1+\rho)^2} \sqrt{\rho(2+\rho)} \right)$$

as a function of ρ . Using the expansion of the function \arccos around the point 1, $\arccos(1 - x) = \sqrt{2x}(1 + \frac{1}{12}x + O(x^2))$, we obtain that, asymptotically for $\rho \ll 1$, $\mathcal{V}_{\text{ovlap}}^* = \frac{8\sqrt{2}}{3} \dot{r}^2 \rho^{3/2} + O(\rho^{5/2})$. The minimal energy \mathcal{E}_* is then given by

$$\mathcal{E}_* = n \pi \dot{r}^2 \left(1 + 2\rho - \frac{8\sqrt{2}}{3\pi} \frac{c(n, 2)}{n} \rho^{3/2} + O(\rho^{5/2}) \right).$$

Example 3.11 (The 3-dimensional case). The theoretical situation in \mathbb{R}^3 is mainly unsolved, with no hope of obtaining an explicit general formula for $c(n, 3)$ in terms of n . The only known exact values are the trivial ones, that is:

$$c(2, 3) = 1, \quad c(3, 3) = 3, \quad c(4, 3) = 6, \quad c(5, 3) = 9.$$

The largest known number of contacts for $n = 6, 7, 8, 9$ are 12, 15, 18, 21, respectively, see [4]. They correspond to clusters which also satisfy the property of being densest packing: the centres of the spheres are the lattice points of a face-centred cubic lattice, see [4, Figure 1].

In [12], the authors study *numerically* the number and the structure of optimal finite-sphere packings – called isoenergetic states – via exact enumeration. They underline the implications for colloidal crystal nucleation.

To conclude this section, we recall the expression of the maximal overlap volume $\mathcal{V}_{\text{ovlap}}^*$ computed in Example 3.7:

$$\mathcal{V}_{\text{ovlap}}^* = 2\pi \dot{r}^3 \rho^2 \left(1 + \frac{2}{3}\rho \right).$$

Therefore, by (3.11), the minimal energy \mathcal{E}_* is given by

$$\mathcal{E}_* = n \frac{4}{3} \pi \dot{r}^3 (1 + \rho)^3 - c(n, 3) 2\pi \dot{r}^3 \rho^2 \left(1 + \frac{2}{3}\rho \right),$$

which leads to the following asymptotic expansion in ρ ,

$$\mathcal{E}_* = n \frac{4}{3} \pi \dot{r}^3 \left(1 + 3\rho + 3 \left(1 - \frac{c(n, 3)}{2n} \right) \rho^2 + O(\rho^3) \right), \quad \rho \ll 1.$$

4 Numerical simulations

We created a companion GitLab page (<https://lab.wias-berlin.de/zass/dynamics-of-spheres>), where the reader can find a Python code we wrote to generate illustrative movies that simulate various planar random dynamics of the type studied in this paper. In particular, we propose illustrations of Section 2 and Section 3.3, that is:

- The two-type dynamics (\mathfrak{S}) of Brownian hard spheres in a Brownian particle bath and their projections on the hard sphere system, for different values of ρ and \dot{z} . The short range of the depletion attraction is clearly visible.
- The dynamics (\mathfrak{S}) of Brownian hard spheres in a Brownian particle bath with high density \dot{z} , which induces a very high stability of the initial hard sphere cluster configuration, close to a maximiser of its contact number.

References

- [1] S. Asakura and F. Oosawa. On interaction between two bodies immersed in a solution of macromolecules. *J. Chem. Phys.*, 22(7):1255–1256, 1954.
- [2] S. Asakura and F. Oosawa. Interaction between particles suspended in solutions of macromolecules. *J. Polym. Sci.*, 33:183–192, 1958.
- [3] K. Bezdek. *Lectures on Sphere Arrangements—The Discrete Geometric Side*, volume 32 of *Fields Institute Monographs*. Springer, New York; Fields Institute for Research in Mathematical Sciences, Toronto, ON, 2013.
- [4] K. Bezdek and M. A. Khan. Contact numbers for sphere packings. In *New Trends in Intuitive Geometry*, volume 27 of *Bolyai Soc. Math. Stud.*, pages 25–47. János Bolyai Math. Soc., Budapest, 2018.
- [5] K. Binder, P. Virnau, and A. Statt. Perspective: The Asakura Oosawa model: A colloid prototype for bulk and interfacial phase behavior. *J. Chem. Phys.*, 141(14):140901, 2014.
- [6] H. Brey and D. G. Kirkpatrick. On the complexity of recognizing intersection and touching graphs of disks. In *Graph Drawing (Passau, 1995)*, volume 1027 of *Lecture Notes in Comput. Sci.*, pages 88–98. Springer, Berlin, 1996.
- [7] K. Burdzy, Z.-Q. Chen, and S. Pal. Archimedes’ principle for Brownian liquid. *Ann. Appl. Probab.*, 21(6):2053–2074, 2011.
- [8] D. Dürr, S. Goldstein, and J. L. Lebowitz. A mechanical model of Brownian motion. *Comm. Math. Phys.*, 78(4):507–530, 1980/81.
- [9] M. Fradon. Stochastic differential equations on domains defined by multiple constraints. *Electron. Commun. Probab.*, 18(26):1–13, 2013.
- [10] M. Fradon and S. Roelly. Infinite system of Brownian balls with interaction: The non-reversible case. *ESAIM Probab. Stat.*, 11:55–79, 2007.
- [11] H. Harborth. Problem 664A. *Elem. Math.*, 29:14–15, 1974.
- [12] R. S. Hoy, J. Harwayne-Gidansky, and C. S. O’Hern. Structure of finite sphere packings via exact enumeration: Implications for colloidal crystal nucleation. *Phys. Rev. E*, 85(5), 2012.
- [13] S. Jansen and D. Tsagkarogiannis. Cluster expansions with renormalized activities and applications to colloids. *Ann. Henri Poincaré*, 21(1):45–79, 2020.
- [14] S. Jansen and D. Tsagkarogiannis. Mayer expansion for the Asakura-Oosawa model of colloid theory. In *Proceedings of the XI International Conference Stochastic and Analytic Methods in Mathematical Physics (Yerevan, 2019)*, volume 6 of *Lectures in pure and applied mathematics*, pages 127–134. Potsdam University Press, 2020.
- [15] K. W. Kratky. The area of intersection of n equal circular disks. *J. Phys. A*, 11:1017–1024, 1978.
- [16] K. W. Kratky. Intersecting disks (and spheres) and statistical mechanics. I. Mathematical basis. *J. Stat. Phys.*, 25(4):619–634, 1981.
- [17] H. N. W. Lekkerkerker and R. Tuinier. Colloids and the depletion interaction. *Lecture Notes in Physics*, 2011.
- [18] H. Ma. Theory and calculation of colloidal depletion interaction. *Int. J. Mod. Phys. B*, 32(18):1840005, 2018.

- [19] R. Roth, R. Evans, and S. Dietrich. Depletion potential in hard-sphere mixtures: Theory and applications. *Phys. Rev. E*, 62:5360–5377, Oct 2000.
- [20] R. Roth and P.-M. König. The depletion potential in one, two and three dimensions. *Pramana J. Phys.*, 64(6):971–980, 2005.
- [21] Y. Saisho and H. Tanemura. On the symmetry of a reflecting Brownian motion defined by Skorohod's equation for a multi-dimensional domain. *Tokyo J. Math.*, 10:419–435, 1987.
- [22] Y. Saisho and H. Tanemura. A Brownian ball interacting with infinitely many Brownian particles in \mathbf{R}^d . *Tokyo J. Math.*, 16(2):429–439, 1993.
- [23] Y. Snir and R. D. Kamien. Entropically driven helix formation. *Science*, 307(5712):1067–1067, 2005.
- [24] A. J. Veretennikov. On strong solutions and explicit formulas for solutions of stochastic integral equations (Russian). *Math. USSR Sbornik*, 111(153)(3):434–452, 1980.
- [25] A. Vrij. Polymers at interfaces and the interactions in colloidal dispersions. *Pure and Appl. Chem.*, 48(4):471–483, 1976.
- [26] R. Wittmann, S. Jansen, and H. Löwen. Geometric criteria for the absence of effective many-body interactions in nonadditive hard particle mixtures. *arXiv:2209.05835*, 2022.