Compensated Integrability and Applications to Mathematical Physics

Denis SERRE

UMPA, UMR 5669 CNRS
École Normale Supérieure de Lyon
France

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Lesson $\#8$ - Hard spheres dynamics

This lesson is devoted to the study of a specific model : that of hard spheres dynamics.

We exploit the DPT constructed in Lesson $\#7.2$, a tensor supported by a graph. We intend to apply the improved Functional Inequality (see Theorem 2 of L$\#7.1$).

We carry our analysis in the case of a large $(10^{23}\,?)$ but finite number N of particles, evolving in the whole space $\mathbb{R}^d$. The one-dimensional case is somewhat trivial so we focus on the situation $d\geq 2$.

The main result is that most of the collisions are grazing, or negligible, in the sense that the transfer of momentum between both particles is very small :

$\longrightarrow \ldots$

Theorem 1

Let N hard spheres evolve in the space $\mathbb{R}^d$. Denote $v_j(t)$ the velocity of the j-th particle. Let $\mathbf{v}$ be the standard deviation of the initial velocities $v_j(0)$. Then we have

$$\sum_{j=1}^{N} TV(t \mapsto v_j(t)) \leq c_d N^2 \mathbf{v}$$

for some universal constant c_d.

The proof is enlightening in that it uses most of the tools at work with Compensated Integrability :

$\longrightarrow \dots$

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- the construction of a non-trivial DPT (done in L#7, Part 2),
- its correction as a Div-controlled tensor,
- the use of the Functional Inequality with determinantal masses (see L#7, Part 1),
- the optimisation of the inequality with respect to parameters,
- a scaling argument.

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State of the art

Denote N the number of particles. In practice, this is a very large number, something like the Avogadro number $6.02 \cdot 10^{23}$.

The initial positions $y_j(0)$ and velocities $v_j(0)$ are given. If m is the mass of an individual particle, we can define the total mass $M = Nm$ and the total energy, a constant of the motion :

$$E(t) := \sum_{j=1}^{N} \frac{m}{2} |v_j(t)|^2 \equiv E_0 := \sum_{j=1}^{N} \frac{m}{2} |v_j(0)|^2.$$

The velocities remain constant between collisions, and the rules governing pairwise collisions are simple ; see L#7.2.

Well-posedness

At first glance, the dynamics seems to be well-posed. However, there remains the possibility that a particle collides simultaneously with two others, or that infinitely many collisions accumulate at some time t^*.

Such configurations do exist. In these situations, it is unclear how the dynamics must be continued. The Cauchy problem is thus not always well-posed.

This is not too much a worry however. In a Master thesis advised by O. Landford, R. K. Alexander[1] proves that for generic initial data, these pathologies do not happen and the dynamics is defined globally in time, in a unique way.

1. R. K. Alexander. *The infinite hard sphere system*. M.S. thesis, University of California at Berkeley (1975).

In a famous talk[2] Ya. Sinai raised the question of whether the collision set is finite. A positive answer was given by Vaserstein[3], whose work was simplified by Illner[4]. Their proofs argued by contradiction and thus did not provide a bound of the number of collisions.

An explicit bound was found a decade later by Burago & all.[5], in the form

$$\#\{\text{collisions}\} \leq (32N^{3/2})^{N^2}.$$

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2. Ya. Sinai. Hyperbolic billiards. *Proceedings of the International Congress of Mathematicians,* (Kyoto 1990), pp 249–260. Math. Soc. Japan, Tokyo (1991).
3. L. N. Vaserstein. On systems of particles with finite-range and/or repulsive interaction. *Commun. Math. Phys.,* **69** (1979), pp 31–56.
4. R. Illner. On the number of collisions in a hard sphere particle system in all space. *Transport Theory and Stat. Phys.,* **18** (1989), pp 71–86.
5. D. Burago, S. Ferleger, A. Kononenko. Uniform estimates on the number of collisions in semi-dispersing billiards. *Annals of Math.,* **147** (1998), pp 695–708.

On the opposite side, Burdzy & Duarte[6] constructed an initial configuration of N hard spheres for which the number of collisions is not less than $\frac{1}{27}\,N^3$. This lower bound was soon improved by Burago & Ivanov[7] in $2^{\lfloor N/2 \rfloor}$.

Thus the collisions might be exponentially many, in terms of the number of particles !

Theorem 1 shows that in this case, most of them display an exponentially small jump $[v]$ of the velocity. It answers the following question raised in B. & I.'s article :

> *It seems that, if the number of collisions is "large", then the overwhelming number of collisions are "inessential" in the sense that they result in almost zero exchange of momenta, energy, and directions of velocities of balls. We will think about it tomorrow.*

6. K. Burdzy, M. Duarte. A lower bound for the number of elastic collisions. *Commun. Math. Phys.*, **372** (2019), pp 679–711.
7. D. Burago, S. Ivanov. Examples of exponentially many collisions in a hard ball system. ArXiv preprint, arXiv :1809.02800v1, 2018.

The mass-momentum tensor

We assume $d \geq 2$ (hence $n \geq 3$) to avoid triviality. We assume a generic initial data, for which the Cauchy problem is globally well-posed, with only pairwise collisions.

Recall (see L#7.2) that the mass-momentum tensor S of the system is the sum of the following contributions :

- For each particle P, whose graph is $\gamma : t \mapsto Y(t)$ (velocity $v = \dot{Y}$), the tensor
$$\frac{1}{\sqrt{1+|v|^2}} \begin{pmatrix} m & mv^T \\ mv & mv \otimes v \end{pmatrix} \mathcal{L}_\gamma,$$
where $\mathcal{L}_\gamma$ is the 1-dimensional Lebesgue measure. We recall that γ is a broken line.
- For every collision between particles (P_i, P_j), the colliton
$$\frac{1}{|[v_i]|} \begin{pmatrix} 0 & 0 \\ 0 & m[v_i] \otimes [v_i] \end{pmatrix} \mathcal{L}_{[x_i^*, x_j^*]},$$
where $x_i^* = (t^*, y_i^*)$ and y_i^* is the position of the particle P_i at collision time t^* ; $[v_i] = -[v_j]$ is the jump of the velocity.

Notice that because of the conservation of energy, the velocities remain uniformly bounded, and therefore the entries of S are finite measures on every strip $(0, T) \times \mathbb{R}^d$. Since S is obviously symmetric and non-negative, and we have shown (Prop 4, L$\#$7.2) that it is divergence-free, it is a DPT over these strips.

Still, a flaw

Applying Compensated Integrability to S is useless. The mass-momentum tensor S is not yet suitable for the following reasons.

- On the one hand, the measure $(\det S)^{\frac{1}{n}}$ vanishes almost everywhere, because S is of rank 0 or 1; apart for the nodes of the graph (collision points x_i^*), but these are not charged by S. Thus the contribution
$$\int_0^T dt \int_{\mathbb{R}^d} (\det S)^{\frac{1}{d}} \, dy$$
is just zero.
- On the other hand, the determinantal masses $\mathrm{Dm}(S; x_i^*)$ (see L#7.1, Definition 1) vanish too.

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To see the latter, remark that at a node x_i^*, S is supported by three <u>coplanar</u> segments, of respective directions

$$V_i = \begin{pmatrix} 1 \\ v_i \end{pmatrix}, \qquad V_i' = \begin{pmatrix} 1 \\ v_i' \end{pmatrix} \quad \text{and} \quad V_i' - V_i = \begin{pmatrix} 0 \\ v_i' - v_i \end{pmatrix}. \qquad (1)$$

Therefore the potential [8] θ depends only upon two independent variables, the coordinates in the plane spanned by V_i, V_i'. Thus the sub-gradient $\partial\theta(x_i^*)$ is a 2-dimensional convex set ; its n-dimensional volume vanishes since $n \geq 3$.

8. Defined in a ball containing only x_i^* and no other node. Recall that $S = \mathrm{D}^2\theta$.

Correctors

To overcome this flaw, we introduce a corrector K, supported in the neighbourhoods of the nodes. Then we apply the Improved Functional Inequality (Thm 2, L#7.1) to the sum $S' := S + K$.

Because the collisions in the strip $(0, T) \times \mathbb{R}^d$ are finitely many, the distance between two nodes is larger than some positive number $2\epsilon > 0$. We may assume that there is no collision at times $t = 0$ and $t = T$, and we choose ϵ smaller than the distance from the nodes to the top and bottom boundaries of the strip.

To begin with, we construct individual correctors K_X at nodes $X = (\tau, Y)$. Notations : v_X / v'_X the incoming/outgoing velocities,

$$V_X = \begin{pmatrix} 1 \\ v_X \end{pmatrix}, \qquad V'_X = \begin{pmatrix} 1 \\ v'_X \end{pmatrix}.$$

We choose an orthonormal basis $(z_3, \dots, z_n)$ of the subspace $\mathrm{Span}(V_X, V'_X)^\perp$.

Consider the segment $\sigma_j = [X - \epsilon z_j, X + \epsilon z_j]$. We define

$$K_X = b_X \sum_{j=3}^{n} z_j \otimes z_j \, \mathcal{L}_{\sigma_j}$$

where $\mathcal{L}_\sigma$ denotes as usual the 1-dimensional Lebesgue measure along σ. The numbers $b_k > 0$ are constants, to be chosen later. Each corrector is obviously symmetric and positive semi-definite.

Because z_j is parallel to σ_j, we know that each $z_j \otimes z_j \, \mathcal{L}_{\sigma_j}$ is Div-controlled, with (see Prop. 1, L#7.2)

$$\mathrm{Div}\,\left(z_j \otimes z_j \, \mathcal{L}_{\sigma_j}\right) = z_j(\delta_{X-\epsilon z_j} - \delta_{X+\epsilon z_j}).$$

We thus have

$$\|\mathrm{Div}\, K_X\|_{\mathcal{M}} = 2(d-1)b_X.$$

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Determinantal masses

Denote $K = \sum K_X$ the sum over all nodes in the strip. The tensor $S' = S + K$ is still supported by a graph. It differs from S in two aspects :

Gain. S' carries a non-trivial determinantal mass at each node X.

Cost. S' is not divergence-free ; we have instead

$$\|\mathrm{Div}\, S'\|_{\mathcal{M}} = 2(d-1) \sum b_X .$$

Let us calculate $\mathrm{Dm}(S'; X)$ at some node, with the same notations as above. By construction, S' is locally block-diagonal according to the splitting

$$\mathbb{R}^n = \mathrm{Span}(V_X, V'_X) \oplus^{\perp} \mathrm{Span}(V_X, V'_X)^{\perp}.$$

In the notations of Proposition 2 (Lesson #7.1), the blocks $S_\pm$ correspond to restrictions of the components S and K_X, respectively. Their sizes are $p = 2$ and $q = n - 2 = d - 1$, hence Prop. 2 gives

$$\mathrm{Dm}(S';X) = \left[\mathrm{Dm}(S_-;X)\mathrm{Dm}(S_+;X)^{d-2}\right]^{\frac{1}{d}}.$$

The easy part is

$$\mathrm{Dm}(S_+;X) = b_X^{\frac{d-1}{d-2}}$$

because $S_+ = K_X$ is the sum of pairwise orthogonal 1-dimensional Lebesgue measures, and $T \mapsto \mathrm{Dm}(T;X)$ is homogeneous of degree $\frac{m}{m-1}$ in dimension m.

The other contribution is calculated *via* Formula (7) of L#7.1. The roles of aX, bY and cZ are played here by $mV_X, -mV'_X$ and $m(V'_X - V_X)$. We have thus

$$\mathrm{Dm}(S_-;X) = \frac{m^2}{4}\,|\det(V_X, V'_X)|,$$

where the determinant has to be taken in the plane spanned by V_X and V'_X. An elementary calculation gives the formula

$$\mathrm{Dm}(S_-;X) = \frac{m^2}{4}\sqrt{\det(v_X, v'_X)^2 + |v'_X - v_X|^2} \geq \frac{m^2}{4}\,|v'_X - v_X|. \quad (2)$$

In conclusion,

$$\mathrm{Dm}(S';X) \geq b_X^{1-\frac{1}{d}}\left(\frac{m^2}{4}\,|v'_X - v_X|\right)^{\frac{1}{d}}.$$

Applying the Improved Functional Inequality

We are now in position to apply Theorem 2 of L#7.1 to S'. Because $(\det S')^{\frac{1}{n}} \equiv 0$, it reduces to

$$\sum_{\text{nodes } X} \mathrm{Dm}(S'; X) \leq \text{ bla-bla.}$$

Here, we get

$$\sum_{\text{nodes}} b_X^{1-\frac{1}{d}} \left(\frac{m^2}{4} \, |v'_X - v_X| \right)^{\frac{1}{d}} \leq c_d \left(\|S'_{\bullet 0}(t=0)\|_{\mathcal{M}} + \|S'_{\bullet 0}(t=T)\|_{\mathcal{M}} + \|\mathrm{Div}\, S'\|_{\mathcal{M}} \right)^{1+\frac{1}{d}}.$$

We already know the value of the last term. For the two others, we remark that on the top and bottom boundaries, we have $S' = S$.

Thanks to Proposition 1 of L#7.2, we have

$$S_{\bullet 0}(t=0) = m \sum_{j=1}^{N} \begin{pmatrix} 1 \\ v_j(0) \end{pmatrix} \delta_{y_j(0)},$$

and the like for $S_{\bullet 0}(t=T)$. Because of the inequality $\sqrt{1+a^2} \le 1 + \frac{a^2}{2}$, we deduce

$$\|S_{\bullet 0}(t=0)\|_{\mathcal{M}} \le M + E_0.$$

Thus IFI gives us

$$\sum_X b_X^{1-\frac{1}{d}} a_X \le c_d \left(2(M+E_0) + 2(d-1) \sum_X b_X \right)^{1+\frac{1}{d}}, \qquad (3)$$

where

$$a_X := \left(\frac{m^2}{4} \, |v'_X - v_X| \right)^{\frac{1}{d}}.$$

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Scaling parameter (1)

So far, (3) is valid for every list of positive parameters b_X. Let us introduce auxiliary parameters, by replacing $b_X = \lambda\beta_X^{\frac{d}{d-1}}$, where λ and β_X are positive. At first glance, this seems unnecessary noise, because we have one more parameter... We rewrite (3) as

$$\sum_X \beta_X a_X \le c'_d \lambda^{\frac{1}{d}-1} \left(M + E_0 + \lambda(d-1)\sum_X \beta_X^{\frac{d}{d-1}} \right)^{1+\frac{1}{d}}.$$

Let us choose the value balancing the contributions in the parenthesis :

$$\lambda = (M+E_0)\left(\sum_X \beta_X^{\frac{d}{d-1}}\right)^{-1},$$

obtaining

$$\sum_X \beta_X a_X \le c''_d (M+E_0)^{\frac{2}{d}} \left(\sum_X \beta_X^{\frac{d}{d-1}}\right)^{\frac{d-1}{d}} = c''_d (M+E_0)^{\frac{2}{d}} \|\vec{\beta}\|_{\ell^{\frac{d}{d-1}}},$$

where $\vec{\beta}$ is the vector of components β_X.

Because ℓ^d is the dual space of $\ell^{\frac{d}{d-1}}$, such an inequality tells us that

$$\|\vec{a}\|_{\ell^d} \leq c_d''(M+E_0)^{\frac{2}{d}}.$$

Rewriting in terms of the velocities, this gives the inequality

$$m^2 \sum_X |[v]| \leq c_d'''(M+E_0)^2.$$

Remarking that the right-hand side does not depend upon the length of the time interval $(0,T)$, we may take the supremum of the left-hand side with respect to T. We obtain therefore

$$m^2 \sum_{j=1}^{N} TV(t \mapsto v_j(t)) \leq c_d'''(M+E_0)^2. \tag{4}$$

Scaling parameter (2)

The above result is still inhomogeneous, physically speaking. This is exactly the same situation as in Lesson #5.
If $\mu > 0$, the scaling $\hat{t} = \mu t, \hat{y} = y$ yields a motion in which the velocities are $\hat{v}_j = \mu v_j$. Applying (4) to this new configuration, we receive the parametrized estimate

$$\mu m^2 \sum_{j=1}^{N} TV(t \mapsto v_j(t)) \leq c_d'''(M + \mu^2 E_0)^2.$$

By choosing $\mu^2 = M/E_0$, we end up with

$$m^2 \sum_{j=1}^{N} TV(t \mapsto v_j(t)) \leq 4c_d''' \sqrt{M^3 E_0}\,,$$

equivalently

$$\sum_{j=1}^{N} TV(t \mapsto v_j(t)) \leq 4c_d''' N^{\frac{3}{2}} \sqrt{\frac{1}{2} \sum_j |v_j(0)|^2}\,. \tag{5}$$

Centering

Our last observation is that (5) is still valid when replacing $v_j(t)$ by $v_j(t)-\bar v$ for some constant vector $\bar v$. This amounts to choosing an inertial moving frame. This does not modified the total variation in the left-hand side, but the right-hand side is changed into

$$4c_d''' N^{\frac{3}{2}}\sqrt{\frac{1}{2}\sum_j |v_j(0)-\bar v|^2}\,.$$

We can minimize it by choosing for $\bar v$ the mean velocity

$$\bar v := \frac{1}{N}\sum_j v_j(0).$$

This leads us to the conclusion

$$\sum_{j=1}^N TV(t\mapsto v_j(t)) \le 4c_d''' N^2 \mathbf{v}, \qquad \mathbf{v} := \sqrt{\frac{1}{N}\sum_j |v_j(0)-\bar v|^2}$$

where $\mathbf{v}$ is the standard deviation. This proves Theorem 1.

Another estimate

We might use (2) in a different way,

$$\mathrm{Dm}(S_-;X)=\frac{m^2}{4}\sqrt{\det(v_X,v_X')^2+|v_X'-v_X|^2}\geq\frac{m^2}{4}\,|\det(v_X,v_X')|.$$

The same calculations yield an estimate of the sum of all the quantities $\frac{1}{2}|\det(v_X,v_X')|$, the areas of triangles whose vertices are $0, v_X$ and v_X'.

Proposition 1

Denote A_j the area swept by the "curve" $t\mapsto v_j(t)$. Then

$$\sum_{j=1}^N A_j\leq c_d N^2 w\mathbf{v}$$

where c_d is a universal constant, and w is the root mean square of the velocity.