Estimating the number and the strength of collisions in molecular dynamics

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Denis Serre
École Normale Supérieure de Lyon*

Abstract

We consider the motion of a finite though large number of particles in the whole space $\mathbb{R}^n$. Particles move freely until they experience pairwise collisions. The class of models include that of hard spheres (Sinai's billiard). We use our recent theory of Compensated Integrability for divergence-controlled positive symmetric tensors in order to estimate how much the particles are deviated by collisions. The only information needed from the initial data is the total mass and the total energy.

1 Models of molecular dynamics

We consider a set of N identical particles of mass m, moving in the whole space $\mathbb{R}^n$. The coordinate in the physical space $\mathbb{R}^{1+n}$ is denoted $x = (t, y)$ where t is the time and $y \in \mathbb{R}^n$ the position.

In practice $n = 3$ and N is of the size of the Avogadro number, but the analysis below is valid in every space dimension and for any cardinality. We shall think of the particles as spheres of radius $a > 0$.

Our assumptions are as follows:

- Each particle P_α has a finite internal energy $\varepsilon_\alpha \geq 0$ and a velocity $v_\alpha \in \mathbb{R}^n$. These parameters remain constant between consecutive collisions involving P_α.
- A collision between two particles $P_{\alpha,\beta}$ occurs when their centers $y_{\alpha,\beta}$ approach to a distance $2a$:
$$|y_\beta - y_\alpha| = 2a.$$
Let us denote $v_{\alpha,\beta}$ and $v'_{\alpha,\beta}$ respectively their velocities before and after the collision. "Approach" is expressed by the inequalities

$$(v_\beta - v_\alpha) \cdot (y_\beta - y_\alpha) < 0, \qquad (v'_\beta - v'_\alpha) \cdot (y_\beta - y_\alpha) \geq 0. \tag{1}$$

*U.M.P.A., UMR CNRS–ENSL # 5669. 46 allée d'Italie, 69364 Lyon cedex 07. France. denis.serre@ens-lyon.fr

- The combined momentum is conserved along the collision:

$$v'_\alpha + v'_\beta = v_\alpha + v_\beta. \tag{2}$$

- The collision is friction-less, meaning that the jump of velocity is orthogonal to the common tangent space to the particles:

$$v'_\alpha - v_\alpha = v_\beta - v'_\beta \parallel y_\beta - y_\alpha. \tag{3}$$

- The combined mechanical energy is conserved along the collision:

$$\frac{m}{2}\left(|v'_\alpha|^2 + |v'_\beta|^2\right) + \varepsilon'_\alpha + \varepsilon'_\beta = \frac{m}{2}\left(|v_\alpha|^2 + |v_\beta|^2\right) + \varepsilon_\alpha + \varepsilon_\beta. \tag{4}$$

The trajectory of a given particle is a polygonal chain. The conservation of energy implies a bound for the emerging velocities:

$$|v'_\alpha|^2 + |v'_\beta|^2 \le |v_\alpha|^2 + \frac{2}{m}\varepsilon_\alpha + |v_\beta|^2 + \frac{2}{m}\varepsilon_\beta.$$

The assumptions made above cover the important case of hard spheres, for which there is no exchange of internal energy (we might as well assume that there is no internal energy at all) and therefore

$$|v'_\alpha|^2 + |v'_\beta|^2 = |v_\alpha|^2 + |v_\beta|^2.$$

In one space dimension ($n = 1$), it covers also the model of *sticky* particles, for which

$$v'_\alpha = v'_\beta = \frac{1}{2}(v_\alpha + v_\beta). \tag{5}$$

Mind however that if $n \ge 2$, the sticky rule (5) is not consistent with (1) as then (3) would write $v_\beta - v_\alpha \parallel y_\beta - y_\alpha$, a property which cannot be ensured in the evolution when $n \ge 2$. Since the friction-less hypothesis is essential for our analysis, the rule (5) must be relaxed in the form

$$v'_\alpha = v_\alpha + \Pi_{y_\beta - y_\alpha}\frac{1}{2}(v_\alpha - v_\beta), \qquad v'_\beta = v_\beta + \Pi_{y_\alpha - y_\beta}\frac{1}{2}(v_\beta - v_\alpha), \tag{6}$$

where Π_y is the orthogonal projection over the line $\mathbb{R}y$. The choice above is the one that minimizes the combined kinetic energy of the outgoing particles, under the friction-less constraint and the conservation of momentum.

Two important quantities emerge from these considerations, namely the total mass $M = Nm$ and the total energy

$$E = \sum_\alpha \left(\frac{m}{2}|v_\alpha(t)|^2 + \varepsilon_\alpha(t)\right),$$

which do not depend on the instant at which they are computed. They are therefore determined by the initial data and we see them as *a priori* given. The third conserved quantity (total momentum)

$$Q = m\sum_\alpha v_\alpha(t)$$

will not be used below, for several reasons. On the first leg its nature is vectorial, which makes it hard to use for an estimate. Besides, it just vanishes if we choose an appropriate inertial frame, a flaw which does not occur to the mass or the energy. Finally, it can be estimated by Cauchy–Schwarz inequality, $|Q| \leq \sqrt{2ME}$, and therefore the knowledge of M and E will always give us a sufficient information.

1.1 Main result

We limit ourselves to the case where every collision involves exactly two particles, and the evolution is defined for every time. For hard spheres, this is a generic situation, as shown by Alexander in his Master thesis [1] ; see Theorem 4.2.1 of [5]. See also Uchiyama's analysis [16] of the Broadwell system, which is a model with a discrete velocity set.

We estimate the number of collisions and their strengths during the whole history, in terms of M and E only. At a collision, each of both particles experiences a change of velocity $v \longmapsto v'$ at a *kink*. The strength of a collision can be expressed as $m|\delta v|$ where $\delta v := v' - v$. We shall measure whether a collision is weak or significant, in terms of the ratio $|\delta v|/\bar{v}$, where

$$\bar{v} := \sqrt{\frac{2E}{M}}$$

is the *characteristic velocity*. At a macroscopic level, where a flow is described by thermodynamical variables, the pressure is intimately related with the number of significant collisions.

In what follows, a *universal constant* c_n is a finite number which may depend upon the space dimension n, but does not depend upon the flow data (initial configuration, total mass M and energy E). The same notation c_n occurs in various places, but the constant may differ from one line to the other.

Theorem 1.1 *Consider a finite system of particles moving in the physical space $\mathbb{R}^n$ according to the laws described above. Let $M = Nm$ be the total mass and $E < \infty$ be the total energy of the system. Let us assume that the collision set is finite on every band $(0,\tau)\times\mathbb{R}^n$, and that the motion involves only binary collisions.*

There exists a universal constant such that the following inequality holds true

$$m^2 \sum_{\text{kinks}} \left(\bar{v}|v'-v| + |v\wedge v'|\right) \leq c_n ME, \tag{7}$$

where the sum runs over the set of kinks.

In other words, we have

$$\sum_{\text{kinks}} |v'-v| \leq c_n N^2 \bar{v}, \qquad \sum_{\text{kinks}} |v \wedge v'| \leq c_n N^2 \bar{v}^2. \tag{8}$$

The inequalities above tell us that if we neglect the *weak* collisions, those for which either $|v'-v| << \bar{v}$ or $|v \wedge v'| << \bar{v}^2$, then the expected number of collisions between two given particles is finite, bounded by a universal constant.

We point out that (8) does not imply the finiteness of the number of collisions. For the hard-spheres model, the question of finiteness was raised by Ya. Sinai [15] and solved by Vaserstein [17], whose work was simplified by Illner [7, 8]. Their proofs argue by contradiction and therefore do not yield an explicit upper bound for the number of collisions. The only known bound was found recently by Burago & al. [2], in the form

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

On the opposite side, Burdzy & Duarte [4] exhibit an initial configuration of N hard spheres for which the number of collisions in the whole history is larger than $\frac{1}{27}N^3$. It is soon improved by Burago & Ivanov [3] in $2^{[\frac{N}{2}]}$ where $[\cdot]$ is the floor function.

The number of collisions can thus be extremely large. Nevertheless, our Theorem 1.1 provides a realistic bound $O(\varepsilon^{-1}N^2)$ for those collisions that have a significant impact on the short-time dynamics, in the sense that $|v'-v| \geq \varepsilon\bar{v}$ for a given threshold $\varepsilon > 0$. This solves a question raised in [3]:

> *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.*

Comments.

- These estimates are independent of the size a of the particles. This was predictible, since a motion of particles of size a yields a similar motion with particle size a' by a change of scale. The number of collisions remains the same.
- The estimates are also independent of the space dimension, apart for the constants c_n.
- In a previous version of this paper, we presented the weaker estimate

$$m^2 \sum_{\text{kinks}} \frac{\bar{v}^2 |v'-v|^2 + |v \wedge v'|^2}{\sqrt{(\bar{v}^2+|v|^2)(\bar{v}^2+|v'|^2)}} \leq c_n ME.$$

  The improvement in (7) is due to an explicit calculation of *determinantal masses* (see Section 4.2), which replaces a coarse lower bound.
- The quantity under the summation in (8.2) can be rewritten $|v| \cdot |v'| \sin\theta$ where θ is the angle by which the trajectory is deviated.

Open questions. A more natural context arises when the gas flows in a bounded domain Ω with impermeable wall. As far as we know, the finiteness of the set of collisions on finite time intervals is still an open question. At least, it is known that for the hard sphere model, a single particle can bounce infinitely many times at the boundary $\partial\Omega$ in finite time. A natural question is to estimate the number and strength of the collisions in a given compact subdomain K. The best that we could expect is that

$$\frac{1}{|J|}\sum_{\text{in}\,J\times K} m|v'-v|$$

be uniformly bounded in terms of $\operatorname{dist}(K,\partial\Omega)$, M and E, when the length of the time interval J is larger than the characteristic time $\operatorname{diam}\Omega/\bar{v}$. So far, we did not succeed to adapt our method in order to establish such a bound. The analogous question arises for a space-periodic flow and remains open as well.

Plan of the paper. The central object of this paper is the *mass-momentum tensor* associated with the motion. Its construction, done in Section 2, is more involved than for flows obeying the Euler or the Boltzmann equations, but the idea is the same: the entries should represent the distribution of mass, momentum and stress. The tensor is a map $x \mapsto T(x)$ taking values in the cone of positive semi-definite matrices $\mathbf{Sym}^+_{1+n}$, albeit a singular one: the entries are bounded measures and their support is one-dimensional. The conservation of mass and momentum is expressed by the row-wise identity $\operatorname{Div} T = 0$. One striking feature in this construction is the introduction of massless virtual particles (*collitons*) whose role is to carry the exchange of momentum between colliding particles. The short Section 3 recalls the principles of Compensated Integrability for divergence-controlled positive tensors, as developped in our former papers [12, 13]. Section 4 is a rather important extension of the theory when such tensors are supported by graphs. Section 5 applies this extended version of Compensated Integrability to a combination of the mass-momentum tensor and an appropriate parametrized complement. An optimal choice of the parameters yields Theorem 1.1.

Acknowledgement. I am indebted to Laure Saint-Raymond and Reinhard Illner for valuable discussions and their help in gathering the relevant literature.

2 The mass-momentum tensor

From now on, we denote $d = 1+n$ the time-space dimension. If J is a line or a segment, we denote δ_J the one-dimensional Lebesgue measure along J. We recall that for a distribution f, positive homogeneity of a given degree κ can be defined either by duality, or by the Euler identity $(x\cdot\nabla)f = \kappa f$. The Lebesgue measure over a k-dimensional linear subspace of $\mathbb{R}^d$ is homogeneous of degree $k-d$; for instance $\mathcal{L}^d$ has degree 0 (obvious), while δ_0 has degree $-d$. If L is a line, or a semi-line, originating from 0, δ_L has degree $1-d$.

2.1 Single particle

We begin by considering a single particle P whose constant velocity is $v \in \mathbb{R}^n$. The trajectory $t \mapsto (t, y(t))$ of the center of mass in the physical space $\mathbb{R}^{1+n}$ is a line L, whose direction is

$$\xi = \frac{V}{|V|}, \qquad \text{where } V := \begin{pmatrix} 1 \\ v \end{pmatrix}.$$

Let us define a symmetric matrix, whose entries are locally finite measures over $\mathbb{R}^{1+n}$, by

$$S = \frac{m}{|V|} V \otimes V \, \delta_L = m|V| \, \xi \otimes \xi \, \delta_L.$$

In other words

$$\langle S_{ab}, \phi \rangle = m V_a \xi_b \int_{\mathbb{R}} \phi(\bar{x} + s\xi) \, ds, \qquad \forall \phi \in C_K(\mathbb{R}^{1+n}),$$

where $\bar{x}$ is an arbitrary point on the line L.

Lemma 2.1 *One has*

$$\operatorname{Div} S = 0,$$

an equation that stands row-wise. More generally, if $Q \in \mathbb{R}^d$ with $Q \neq 0$, and $\eta = \frac{Q}{|Q|}$, then for every line $L = \bar{x} + \mathbb{R}\eta$, the symmetric tensor

$$S^Q := Q \otimes \eta \, \delta_L$$

is divergence-free.

Notice that for a particle, S is nothing but S^Q with $Q = mV$. Remark also that S^Q is everywhere positive semi-definite.

Proof
If ϕ is a test function, then

$$\langle \operatorname{Div} S^Q, \phi \rangle = -\langle S^Q, \nabla \phi \rangle = -Q \int_{\mathbb{R}} \eta \cdot \nabla \phi(\bar{x} + s\eta) \, ds = -Q \int_{\mathbb{R}} \frac{d}{ds} \phi(\bar{x} + s\eta) \, ds = 0.$$

■

2.2 Multi-line configuration

When L is replaced by a semi-infinite line $L^+ = \bar{x} + \mathbb{R}_+ \eta$, the tensor

$$S^{Q+} := Q \otimes \eta \, \delta_{L^+}$$

is no longer divergence-free. The calculation above yields

$$\langle \operatorname{Div} S^{Q+}, \phi \rangle = \phi(\bar{x}) Q, \tag{9}$$

which is recast as

$$\mathrm{Div}\, S^{Q+} = Q\,\delta_{\bar{x}}.$$

Now, if finitely many vectors $Q_1, Q_2, \ldots$ are given, together with a point $\bar{x} \in \mathbb{R}^d$, we may form the converging semi-lines $L_j^+ = \bar{x} + \mathbb{R}_+ Q_j$ and define a symmetric tensor

$$S_{\mathrm{mult}} := \sum_j S^{Q_j+}.$$

Then (9) tells us that S_{mult} is divergence-free whenever

$$\sum_j Q_j = 0. \tag{10}$$

Application to 1-D molecular dynamics. When $n = 1$, we may simplify the model by setting $a = 0$. At a binary collision, the point particles meet at some point $\bar{x} \in \mathbb{R}^{1+1}$, with incoming velocities v, w and outgoing ones v', w'. Let us choose

$$V_1 = -\begin{pmatrix} 1 \\ v \end{pmatrix}, \qquad V_2 = -\begin{pmatrix} 1 \\ w \end{pmatrix}, \qquad V_3 = \begin{pmatrix} 1 \\ v' \end{pmatrix}, \qquad V_4 = \begin{pmatrix} 1 \\ w' \end{pmatrix} \tag{11}$$

and $Q_j = mV_j$. Then the positive semi-definite tensor

$$S^{Q_1+} + S^{Q_2+} + S^{Q_3+} + S^{Q_4+}$$

associated with this pair of particles is divergence-free ; the compatibility condition $Q_1 + Q_2 + Q_3 + Q_4 = 0$ is ensured by the conservation of mass and momentum through the collision. Its support is the union of the trajectories.

2.3 Binary collisions ($n \geq 2$)

When $n \geq 2$ instead, the radius a must be positive, in order that collisions take place.

Let two particles P_i and P_j collide at some time t^*. The trajectory of P_i displays a kink at a point $\bar{x}_i = (t^*, \bar{y}_i)$, and that of P_j does at $\bar{x}_j = (t^*, \bar{y}_j)$ at the same instant t^*. We have $|\bar{y}_j - \bar{y}_i| = 2a$. Let us define $V_1, \ldots, V_4$ as in (11). Locally, the trajectories are made of segments of the semi-lines

$$L_1^+ = \bar{x}_i + \mathbb{R}_+ V_1, \qquad L_2^+ = \bar{x}_j + \mathbb{R}_+ V_2, \qquad L_3^+ = \bar{x}_i + \mathbb{R}_+ V_3, \qquad L_4^+ = \bar{x}_j + \mathbb{R}_+ V_4.$$

Let us denote again $Q_j = mV_j$. Because the lines do not meet at a single point, the tensor $S = S^{Q_1+} + S^{Q_2+} + S^{Q_3+} + S^{Q_4+}$ is not divergence-free. We have instead

$$\mathrm{Div}\, S = (Q_1 + Q_3)\delta_{x_i} + (Q_2 + Q_4)\delta_{x_j} = (Q_1 + Q_3)(\delta_{x_i} - \delta_{x_j}).$$

In order to recover a divergence-free tensor, we introduce a vector Q

$$Q = \begin{pmatrix} 0 \\ q \end{pmatrix}, \qquad q = m(v' - v) = m(w - w').$$

Because of (3), the segment $C=[\bar{x}_i,\bar{x}_j]$ has direction Q. In the neighbourhood of the collision, we can define the tensor

$$T=S^{Q_1+}+S^{Q_2+}+S^{Q_3+}+S^{Q_4+}+Q\otimes\eta\,\delta_C.$$

Each of the five terms in the sum above is divergence-free away from either $\bar{x}_i$ or $\bar{x}_j$. At $\bar{x}_i$, $\operatorname{Div}T$ is a sum of three Dirac masses, whose weight is

$$m(V_1+V_3)-Q=\begin{pmatrix}-m+m-0\\ -mv+mv'-q\end{pmatrix}=0, \tag{12}$$

where the minus sign in front of Q comes from the fact that Q is oriented from x_j to x_i. A similar identity holds true at $\bar{x}_j$, with now a plus sign in front of Q. We conclude that

$$\operatorname{Div}T=0.$$

We may interpret the contribution $Q\otimes\eta\,\delta_C$ as that of a virtual particle. This particle is massless, because the first component of Q vanishes. It carries the momentum which is exchanged instantaneously between P_i and P_j. We suggest the name *colliton* for this object. If we took in account relativistic effects, there would be instead a pair of virtual particles (a particle and its anti-particle), travelling at the speed of light.

2.4 The complete construction

Assuming again that only binary collisions occur, we consider the union of trajectories of the centers of the N particles. Each trajectory is a polygonal chain whose kinks occur where and when the particle suffers a collision. Each segment J of a trajectory between two consecutive collisions contributes, as explained above, with the tensor

$$mV\otimes\xi\,\delta_J,\qquad V=\begin{pmatrix}1\\ v\end{pmatrix},\qquad \xi=\frac{V}{|V|},$$

where v is the particle velocity along J. At a collision we also have the contribution of the corresponding colliton, as described in the previous paragraph. The sum T of all these contributions is a divergence-free positive semi-definite tensor, which we call the *mass-momentum* tensor of the configuration.

We point out that the support of T is a graph, a one-dimensional object in $\mathbb{R}^{1+n}$. Thus T vanishes almost everywhere in the Lebesgue sense. The support can be equiped with the positive measure $\operatorname{Tr}T$, with respect to which T is rank-1 almost everywhere.

Finiteness. Because the particles are finitely many, and the collisions are finitely many in every band $H_\tau=(0,\tau)\times\mathbb{R}^n$ by assumption, the restriction of the entries of T to H_τ are finite measures. This property is an essential hypothesis in Compensated Integrabillity (Theorem 3.1 below). Remark however that we do not have a practical bound of the total mass of T in H_τ, because we do not control efficiently the number and the strength of the collitons. This flaw is the reason why we could not extend Theorem 1.1 to flows in a bounded domain or in the torus.

3 Compensated integrability

We shall make use of our recent theory of Compensated Integrability for divergence-controlled positive symmetric tensors, for which we refer to [12, 13]. The appropriate version is given in the theorem below. Let $U \subset \mathbb{R}^d$ be an open set. Let S be a distribution over U that takes values in the cone $\mathbf{Sym}_d^+$. By positiveness, the entries S_{ab} are locally finite measures. We say that S is *divergence-controlled* if these entries, as well as the coordinates of $\mathrm{Div}\, S$ are finite measures. We recall that a divergence-controlled tensor admits a normal trace $S\vec{\nu}$ along the boundary ∂U, which *a priori* belongs to the dual space of $\mathrm{Lip}(\partial U)$.

We denote $\|\mu\|$ for the total mass of a (vector-valued) bounded measure μ,

$$\|\mu\| = \langle |\mu|, \mathbf{1} \rangle.$$

This notation applies below in two distinct contexts, whether μ is a measure over an $(n+1)$-dimensional slab $H = (t_-, t_+) \times \mathbb{R}^n$, or a measure over $\mathbb{R}^n$.

Theorem 3.1 *Let $H = (t_-, t_+) \times \mathbb{R}^n$ be a slab in $\mathbb{R} \times \mathbb{R}^n$, and S be symmetric positive semi-definite tensor defined over H. We assume that S is divergence-controlled in H. Finally we assume that the normal traces $S\vec{e}_t$ at the initial and final times $t = t_\pm$ are themselves bounded measures.*

Then $(\det S)^{\frac{1}{n+1}}$ belongs to $L^{1+\frac{1}{n}}(H)$ and we have

$$\int_H (\det S)^{\frac{1}{n}} dy\, dt \le c_n \left(\|S\vec{e}_t(t_-)\| + \|S\vec{e}_t(t_+)\| + \|\mathrm{Div}\, S\| \right)^{1+\frac{1}{n}}, \tag{13}$$

where c_n is a finite constant independent of S and H.

Remarks.

- The constant in Theorem 3.1 is
$$\frac{1}{(n+1)|S_n|^{\frac{1}{n}}},$$
where S_n is the unit sphere in $\mathbb{R}^{1+n}$. The combination of (13) with other inequalities will yield various functional inequalities where different constants, still denoted c_n, will occur. These constants, which can be computed explicitly, are of moderate size. A uniform upper bound such as $c_n \le 10$ seems plausible.

- The additional assumption that the normal traces are bounded measures is equivalent to saying that the extension $\tilde{S}$ by 0_{1+n} away from H enjoys too the property that $\mathrm{Div}\, \tilde{S}$ is a bounded measure. Then
$$\mathrm{Div}\, \tilde{S} = \widetilde{\mathrm{Div}\, S} - S\vec{e}_t(t_-) \otimes \delta_{t=t_-} + S\vec{e}_t(t_+) \otimes \delta_{t=t_+}$$

- The qualitative part of the theorem is that the bounded measure $(\det S)^{\frac{1}{d}}$ is absolutely continuous with respect to the Lebesgue measure, and that its density is a function of class $L^{\frac{d}{d-1}}$, where $\frac{d}{d-1} = 1 + \frac{1}{n}$. The quantitative part (13) estimates this density.

- This theorem is useless when S is rank-1 almost everywhere ; one has $(\det S)^{\frac{1}{d}} \equiv 0$ and the estimate (13) is trivial. The goal of the next section is to improve the statement when the tensor is supported by a graph.

4 Tensors supported by a graph

Let G be a non-oriented graph included in H. Let S be a tensor of the form

$$S = \sum_J a_J \eta_J \otimes \eta_J \delta_J, \tag{14}$$

where the sum runs over the edges. The unit vector $\pm\eta_J$ is the direction of J, and $a_J > 0$ is a weight of the edge. We already know that

$$\mathrm{Div}\, S = \sum_w m(w)\delta_w$$

where the sum runs over the vertices and the weight is given by

$$m(w) = \sum_{J \sim w} a_J \eta_J.$$

This sum runs over the edges around the vertex w, with η_J oriented outward.

The tensor S is positive semi-definite, its entries being locally finite measures. The divergence is a finite measure too, as well as the normal traces at $t = t_\pm$. For instance

$$S\vec{e}_t(t_-) = \sum{}' a_J \eta_J$$

where the sum runs over the set of edges that meet the hyperplane $t = t_-$.

When applying Theorem 3.1, we have therefore a good control of the right-hand side. Unfortunately, it is of no help as the left-hand side vanishes identically, due to $\det S \equiv 0$. We shall see however that something can be gained at those vertices where $m(w) = 0$ (S is locally divergence-free), provided that the set of directions $\{\eta_J : J \sim w\}$ span $\mathbb{R}^d$.

4.1 Minkowski potentials

To begin with, we recall that if $U \subset \mathbb{R}^d$ is a convex open subset and $\theta \in W^{2,d-1}(U)$ is given, then the cofactor matrix $\Lambda^\theta := \widehat{\mathrm{D}^2\theta}$ of the Hessian is symmetric, integrable and divergence-free. If in addition θ is convex, then the tensor is positive semi-definite. Because of the formula

$$\det \widehat{R} = (\det R)^{d-1}$$

for $d \times d$ matrices, the expression

$$\int_U (\det \Lambda^\theta)^{\frac{1}{d-1}} dx$$

which is at stake in Compensated Integrability equals

$$\int_U \det \mathrm{D}^2\theta \, dx = \mathrm{vol}(\nabla\theta(U)).$$

The Sobolev regularity of the potential can actually be lowered, and one can show that every convex θ yields a non-negative divergence-free tensor Λ^θ. Of special interest is the case where θ is positively homogeneous of degree 1 (for instance, θ might be a norm). Then Λ^θ is positively homogeneous of degree $1-d$,

$$\Lambda^\theta = \mu^\theta\left(\frac{x}{|x|}\right)\frac{x\otimes x}{|x|^{d+1}},$$

where μ^θ is some positive finite measure over the unit sphere. This measure satisfies the relation

$$\int_{S_{d-1}} e\mu^\theta(e) = 0.$$

Mind that when $\theta \in W^{2,d-1}_{\mathrm{loc}}$, μ^θ is just an integrable function.

Conversely, if μ is positive measure over S_{d-1}, one may form the positive symmetric tensor

$$\Lambda = \mu\left(\frac{x}{|x|}\right)\frac{x\otimes x}{|x|^{d+1}}, \tag{15}$$

which turns out to be divergence-free if and only if

$$\int_{S_{d-1}} e\mu(e) = 0. \tag{16}$$

The problem of whether there exists a convex potential θ, positively homogeneous of degree 1, such that $\Lambda = \Lambda^\theta$ received a positive answer, given by Pogorelov [10]. The solution exists and is unique, up to the addition of a linear form. When the support of μ spans $\mathbb{R}^d$, this problem is equivalent to that of Minkowski, which asks for a convex body whose Gaussian curvature (here μ) is prescribed as a function of the unit normal. For this reason, we call θ the *Minkowski potential* of Λ (or of μ).

The special case where μ is a fiinite sum of Dirac masses is precisely that solved by Minkowski himself [9], then the body is a convex polytope.

4.2 Determinantal mass at a vertex

Let S be a divergence-controlled positive semi-definite symmetric tensor over H, and suppose that in a neighbourhood U of some point x^*, it is of the form (14) for finitely many edges attached to x^*. Assume also that S is divergence-free in this neighbourhood, that is $m(x^*) = 0$.

Up to a translation, we may set $x^* = 0$. Then S is locally homogeneous of degree $1-d$, and the equation $m(0) = 0$ just says that S fulfills condition (16). By Pogorelov's theorem, it can therefore be parametrized locally as $S = \Lambda^\theta$ for some convex function, positively homogeneous of degree 1.

We now smooth out θ in a ball B such that $2B \subset U$. The resulting potential ξ is C^∞ in B and coincides with θ in $2B \setminus B$; we point out that ξ is no longer positively homogeneous. The associated tensor Λ^ξ is C^∞ in B and coincides with Λ^θ in $2B \setminus B$. Thus we may form the divergence-controlled tensor $\tilde{S}$ such that $\tilde{S} = S$ in $H \setminus B$ and $\tilde{S} = \Lambda^\xi$ in $2B$. We have $\mathrm{Div}\,\tilde{S} = \mathrm{Div}\,S$ because both vanish in $2B$. Besides, the normal traces at $t = t_\pm$ coincide. When applying (13) to $\tilde{S}$, the right-hand side is therefore unchanged. However, the left-hand side gains the contribution

$$\int_B (\det \Lambda^\xi)^{\frac{1}{d-1}} dy\, dt = \int_B \det \mathrm{D}^2 \xi \, dy\, dt = \mathrm{vol}(\nabla \xi(B)).$$

The latter quantity is precisely the volume of the convex body[1] enclosed by the boundary $\nabla\theta(S_{d-1})$. We call it the *determinantal mass* of S at the vertex and denote it $\mathrm{Dm}(S;x^*)$. We now apply Estimate (13) to $\tilde{S}$ and obtain

$$\begin{aligned}
\int_H (\det S)^{\frac{1}{n}} dy\, dt + \mathrm{Dm}(S;x^*) &= \int_H (\det \tilde{S})^{\frac{1}{n}} dy\, dt \\
&\le c_n \left(\|\tilde{S}\vec{e}_t(t_-)\| + \|\tilde{S}\vec{e}_t(t_+)\| + \|\mathrm{Div}\,\tilde{S}\| \right)^{1+\frac{1}{n}} \\
&= c_n \left(\|S\vec{e}_t(t_-)\| + \|S\vec{e}_t(t_+)\| + \|\mathrm{Div}\,S\| \right)^{1+\frac{1}{n}}.
\end{aligned}$$

More generally, applying the construction described above at every vertex where S is graph-like and divergence-free, we obtain the following improvement of Theorem 3.1.

Theorem 4.1 *Let $H = (t_-, t_+) \times \mathbb{R}^n$ be a slab in $\mathbb{R} \times \mathbb{R}^n$, and S be a symmetric, positive semi-definite tensor defined over H. We assume that S is divergence-controlled and that the normal traces $S\vec{e}_t$ at the initial and final times $t = t_\pm$ are bounded measures too.*

Then we have

$$\int_H (\det S)^{\frac{1}{n}} dy\, dt + \sum \mathrm{Dm}(S;x^*) \le c_n \left(\|S\vec{e}_t(t_-)\| + \|S\vec{e}_t(t_+)\| + \|\mathrm{Div}\,S\| \right)^{1+\frac{1}{n}}, \tag{17}$$

where the summation extends over the vertices $x^* \in H$ about which S is of the form (14) and is divergence-free.

Remarks.

- The calculation above suggests to redefine $(\det S)^{\frac{1}{d-1}}$ as the sum of an absolutely continuous part, the one at stake in Theorem 3.1, and a singular one, made of Dirac masses $\mathrm{Dm}(S;x^*)\,\delta_{x^*}$ at every point x^* where S is graph-like and divergence-free.
- The map $S \mapsto \mathrm{Dm}(S;x^*)$ is homogeneous of degree $\frac{d}{d-1}$, invariant under the action of the orthogonal group: if R is a rotation and S is given by (14), then $\mathrm{Dm}(S;x^*) = \mathrm{Dm}(S^R;x^*)$, where S^R is defined by rotating each of the η_J's and keeping x^* and a_J unchanged.

[1] This is the solution of Minkowski's problem.

- There is nothing special in the choice of a slab. Theorem 4.1 has a version in an arbitrary bounded open domain $\Omega\subset\mathbb{R}^d$.
- The calculation above is easily adapted in the case where S is only divergence-controlled. For instance, if S is divergence-free at x^* and ϕ is a smooth function, Compensated Integrability applied to ϕS is valid with a contribution $\phi(x^*)^{\frac{d}{d-1}}\mathrm{Dm}(S;x^*)$.
- A determinantal mass $\mathrm{D}(S;x^*)$ can actually be defined whenever S is locally homogeneous of degree $1-d$. Below, we need only the case treated in Theorem 4.1. We actually use only simple cases where the Minkowski potential and its determinantal mass can be calculated explicitly, see the next Section.

4.3 Calculations of determinantal masses

We do not know of a closed form of $\mathrm{Dm}(S;x^*)$ in terms of the measure μ. We present here two useful situations where such a calculation is possible.

4.3.1 The planar case

When $d=2$ (that is $n=1$), we do have a closed formula, associated with the linearity of the operator $\theta\mapsto\widehat{\mathrm{D}^2\theta}$.

Proposition 4.1 **($d=2$)** *Let μ be a positive measure over the unit circle S_1 satisfying the constraint (16). Let Λ be the divergence-free tensor defined over $\mathbb{R}^2$ by (15). Then the Minkowski potential of Λ is given by*

$$\theta(x)=|x|\,p\left(\frac{x}{|x|}\right),$$

where p is a 2π-periodic solution of $p+p''=\mu$ (the derivatives are taken with respect to angle).

The determinantal mass of Λ at the origin is given by

$$\mathrm{Dm}(\Lambda;0)=\frac18\int_0^{2\pi}\int_0^{2\pi}\mu(s_1)\mu(s_2)\sin|s_2-s_1|\,ds_1ds_2. \tag{18}$$

We point out that (16), which writes here

$$\int_0^{2\pi}\mu(s)\sin s\,ds=\int_0^{2\pi}\mu(s)\cos s\,ds=0,$$

is precisely the solvability condition of $p+p''=\mu$ in the realm of periodic functions.

We shall use the following consequence of Proposition 4.1.

Corollary 4.1 *Let $V,W,Z \in \mathbb{R}^2$ be given, such that $V+W+Z=0$. For some $x^* \in \mathbb{R}^2$, we consider the divergence-free tensor*

$$\Lambda := \frac{V\otimes V}{|V|}\,\delta_{x^*+\mathbb{R}_+V} + \frac{W\otimes W}{|W|}\,\delta_{x^*+\mathbb{R}_+W} + \frac{Z\otimes Z}{|Z|}\,\delta_{x^*+\mathbb{R}_+Z}.$$

We have

$$\mathrm{Dm}(\Lambda;x^*) = \frac{1}{4}\,|\det(V,W)|. \tag{19}$$

Mind that this expression is symmetric in V,W,Z. For instance,

$$\det(V,Z) = \det(V,-V-W) = -\det(V,W).$$

Actually, if we label V,W,Z in the trigonometric order, with arguments $0\le\alpha<\beta<\gamma<2\pi$, the measure μ is given by

$$\mu = |V|\delta_\alpha + |W|\delta_\beta + |Z|\delta_\gamma,$$

and the formula (18) gives

$$\begin{aligned}\mathrm{Dm}(\Lambda;x^*) &= \frac{1}{4}(|V|\cdot|W|\,\sin(\beta-\alpha)+|W|\cdot|Z|\,\sin(\gamma-\beta)+|Z|\cdot|V|\,\sin(\gamma-\alpha))\\ &= \frac{1}{4}\,(|\det(V,W)|+|\det(W,Z)|-|\det(Z,V)|) = \frac{1}{4}\,|\det(V,W)|,\end{aligned}$$

where we have used $\beta-\alpha, \gamma-\beta \in (0,\pi)$ and $\gamma-\alpha\in(\pi,2\pi)$.

Proof (of Proposition 4.1.)

Let θ be the Minkowski potential of Λ and p be its restriction to the unit circle. An elementary calculation yields

$$\Lambda = \widehat{\mathrm{D}^2\theta} = \begin{pmatrix}\theta_{,22} & -\theta_{,12}\\ -\theta_{,12} & \theta_{,11}\end{pmatrix} = (p+p'')\,\frac{x\otimes x}{|x|^3}\,,$$

whence the differential equation $p+p''=\mu$. As mentionned above, there exists a 2π-periodic solution p because of the constraints (16) which express the divergence-freeness of Λ. The solution is unique up to the addition of $a\sin+b\cos$; in terms of θ, this means uniqueness up to the addition of a linear form. The image of $\nabla\theta$ is the curve

$$\phi \longmapsto \begin{pmatrix}p(\phi)\cos\phi - p'(\phi)\sin\phi\\ p(\phi)\sin\phi + p'(\phi)\cos\phi\end{pmatrix}.$$

The mass $\mathrm{Dm}(\Lambda;0)$, being the area enclosed by this curve, equals

$$\begin{aligned}\mathrm{Dm}(\Lambda;0) &= \frac{1}{2}\int_0^{2\pi}\theta_{,1}d\theta_{,2} = \frac{1}{2}\int_0^{2\pi}(p\cos\phi-p'\sin\phi)(p+p'')\cos\phi\,d\phi\\ &= \frac{1}{2}\int_0^{2\pi}(p\cos\phi-p'\sin\phi)\mu\cos\phi\,d\phi.\end{aligned}$$

Let us define

$$\lambda(\phi) := \int_0^\phi \mu(s)\cos s\,ds,$$

which is periodic because of (16). Then

$$\begin{aligned}\mathrm{Dm}(\Lambda;0) &= \frac{1}{2}\int_0^{2\pi}(p\cos\phi - p'\sin\phi)\lambda'\,d\phi = \frac{1}{2}\int_0^{2\pi}(p+p'')\lambda\sin\phi\,d\phi = -\frac{1}{2}\int_0^{2\pi}\mu\lambda\sin\phi\,d\phi \\ &= -\frac{1}{2}\int_0^{2\pi}d\phi\int_0^\phi \mu(\phi)\mu(s)\sin\phi\cos s\,ds.\end{aligned}$$

Using again (16), this gives

$$\mathrm{Dm}(\Lambda;0) = \frac{1}{2}\int_0^{2\pi}d\phi\int_\phi^{2\pi}\mu(\phi)\mu(s)\sin\phi\cos s\,ds.$$

Instead, we may use Fubini, to have

$$\mathrm{Dm}(\Lambda;0) = -\frac{1}{2}\int_0^{2\pi}ds\int_s^{2\pi}\mu(\phi)\mu(s)\sin\phi\cos s\,d\phi \overset{\text{relabel.}}{=\!=} -\frac{1}{2}\int_0^{2\pi}d\phi\int_\phi^{2\pi}\mu(\phi)\mu(s)\sin s\cos\phi\,ds.$$

Combining the last two lines, we have

$$\mathrm{Dm}(\Lambda;0) = \frac{1}{4}\int_0^{2\pi}d\phi\int_\phi^{2\pi}\mu(\phi)\mu(s)\sin(\phi - s)\,ds,$$

which by symmetrization, yields (18).

■

4.3.2 Direct sums

We continue our study of tensors of the form (14), say centered at the origin. We suppose here that the set of vectors η_J can be split into two subsets, orthogonal to each other. In other words, $\mathbb{R}^d$ splits as $E_- \oplus^\perp E_+$, so that each η_J is either in E_- or in $E_+ = E_-^\perp$. Up to a rotation, we may always assume that $E_- = \mathbb{R}^p \times \{0\}$ and $E_+ = \{0\} \times \mathbb{R}^q$ with $p+q=d$. Our tensor writes therefore blockwise

$$S = \begin{pmatrix} S_- \otimes \delta_{x_+=0} & 0 \\ 0 & \delta_{x_-} \otimes S_+ \end{pmatrix}. \tag{20}$$

The tensors $S_\pm$ are defined over open subsets of $E_\pm$ and inherit the divergence-freeness. They are actually of a form similar to (14), though in either $\mathbb{R}^p$ or $\mathbb{R}^q$ instead of $\mathbb{R}^d$. Each of both admits a Minkowski potential:

$$S_- = \widehat{\mathrm{D}_-^2\theta_-}, \qquad S_+ = \widehat{\mathrm{D}_+^2\theta_+}$$

where $\theta_\pm$ is a convex function of $x_\pm$, positively homogeneous of degree 1. The derivative D_- (resp. D_+) acts over the coordinates in E_- (resp. E_+).

Lemma 4.1 *We assume* $\mathrm{Dm}(S_-,0),\mathrm{Dm}(S_+,0)>0$. *The Minkowski potential of the divergence-free tensor S given in (20) is*

$$\theta(x_-,x_+)=a_-\theta_-(x_-)+a_+\theta_+(x_+)$$

where

$$a_-=(\mathrm{Dm}(S_-,0))^{-\frac{q}{d-1}}(\mathrm{Dm}(S_+,0))^{\frac{q-1}{d-1}},\qquad a_+=(\mathrm{Dm}(S_-,0))^{\frac{p-1}{d-1}}(\mathrm{Dm}(S_+,0))^{-\frac{p}{d-1}}. \tag{21}$$

Corollary 4.2 *The determinantal masses of* S,S_- *and* S_+ *satisfy the relation*

$$\mathrm{Dm}(S,0)=(\mathrm{Dm}(S_-,0))^{\frac{p-1}{d-1}}(\mathrm{Dm}(S_+,0))^{\frac{q-1}{d-1}}. \tag{22}$$

Proof

We look for a potential θ given as a linear combination of θ_- and θ_+, where we have to identify the coefficients $a_\pm$.

Because the calculation of determinantal masses requires an approximation procedure (to smooth out the vertex singularity of the potential), we begin by considering smooth convex functions $\xi_\pm$ over $\mathbb{R}^p$ and $\mathbb{R}^q$, instead of $\theta_\pm$. We have easily

$$\widehat{a_-\xi_-+a_+\xi_+}=\begin{pmatrix} a_-^{p-1}a_+^q(\det \mathrm{D}_+^2\xi_+)\widehat{\mathrm{D}_-^2\xi_-} & 0 \\ 0 & a_-^p a_+^{q-1}(\det \mathrm{D}_-^2\xi_-)\widehat{\mathrm{D}_+^2\xi_+}\end{pmatrix}.$$

When ξ_- converges uniformly to θ_-, $\det \mathrm{D}_-^2\xi_-$ tends towards the mesure $\mathrm{Dm}(S_-;0)\,\delta_{x_-=0}$ while $\widehat{\mathrm{D}_-^2\xi_-}$ tends to S_-. Passing to the limit, we infer

$$\widehat{a_-\theta_-+a_+\theta_+}=\begin{pmatrix} a_-^{p-1}a_+^q\mathrm{Dm}(S_+;0)\,S_-\otimes\delta_{x_+=0} & 0 \\ 0 & a_-^p a_+^{q-1}\mathrm{Dm}(S_-;0)\,\delta_{x_-=0}\otimes S_+\end{pmatrix}.$$

We recover the tensor S by chosing the solution (a_-,a_+) of the system

$$a_-^{p-1}a_+^q\mathrm{Dm}(S_+;0)=1,\qquad a_-^p a_+^{q-1}\mathrm{Dm}(S_-;0)=1.$$

This gives us the formulæ (21).

Finally, the body enclosed by the image of $\nabla(a_-\theta_-+a_+\theta_+)$ is the Cartesian product of the bodies enclosed by the images of $a_\pm\nabla_\pm\theta_\pm$ respectively. In terms of volumes, we have therefore

$$\mathrm{Dm}(S;0)=a_-^p a_+^q\mathrm{Dm}(S_-,0)\cdot\mathrm{Dm}(S_+;0),$$

which gives the relation (22).

■

Remarks.

- Formula (22) is a rather natural generalization of the identity $\det M = \det M_- \times \det M_+$ for a block diagonal matrix.
- The procedure above can be extended to the situation where $\mathbb{R}^d$ is split into an arbitrary number of orthogonal subspaces whose union contains the η_J's.
- The orthogonality between E_- and E_+ is not an essential ingredient, because it is always possible to make a linear change of variable which maps isometrically E_- over $\mathbb{R}^p \times \{0\}$ and E_+ over $\{0\} \times \mathbb{R}^d$, and to modify T accordingly (see [12]). The general formula (22) will however contain a factor reflecting the angle between E_- and E_+.

The simplest example of a direct sum is certainly given by the potential

$$\theta_{\rm abs}(x) = \sum_1^d |x_j| = \|x\|_1.$$

The corresponding tensor is diagonal

$$\Lambda_{\rm abs} = \sum_1^d \vec{e}_j \otimes \vec{e}_j \, \delta_{\mathbb{R}\vec{e}_j} = \begin{pmatrix} \delta_{\hat{x}_1=0} & & \\ & \ddots & \\ & & \delta_{\hat{x}_d=0} \end{pmatrix},$$

where as usual $\hat{x}_j = (x_, \dots, x_{j-1}, x_{j+1}, \dots, x_d) \in \mathbb{R}^{d-1}$. We have immediately

$$\mathrm{Dm}(\Lambda_{\rm abs}; 0) = 2^d. \tag{23}$$

5 The binary estimate in the whole space

This section is devoted to the proof of Theorem 1.1. The physical domain is $\mathbb{R}^n$. We consider a flow in which the collisions form a discrete set and are only binary. We assume without loss of generality that there is no collision at the initial time. We denote T the mass-momentum tensor constructed in Section 2.

To begin with, we choose a time $\tau > 0$ at which there is no collision and we set $H_\tau = (0, \tau) \times \mathbb{R}^n$.

A complement to the mass-momentum tensor. Let K be a kink of a trajectory, happening at a point $x^* \in H_\tau$. The incoming/outgoing velocities of the particle under consideration being v, v' respectively, with $v' \neq v$, we complete the free family

$$V = \begin{pmatrix} 1 \\ v \end{pmatrix}, \quad V' = \begin{pmatrix} 1 \\ v' \end{pmatrix}$$

into a basis $(V, V', z_2, \dots, z_n)$ of $\mathbb{R}^{1+n}$. Here $(z_2, \dots, z_n)$ is some orthonormal basis of $\mathrm{Span}(V, V')^\perp$. We define the positive semi-definite tensor

$$S_K = \sum_{j=2}^{n} z_j \otimes z_j \delta_{\sigma_j},$$

where $\sigma_j := (x^* - \varepsilon_K z_j, x^* + \varepsilon_K z_j)$ is a segment, small enough that it be contained in H_τ. Mind that the vectors z_j do depend on the kink, even if it is not explicit in our notation. The lengths $\varepsilon_K > 0$ are chosen small enough that the corresponding segments are contained in H_τ, do not overlap and do not intersect the support of T away from the kinks. Because the number of collisions is finite in H_τ, the entries of S are finite measures.

We form an auxiliary tensor

$$T' = T + S, \qquad S := \sum_{\text{kinks in } H_\tau} b_K S_K,$$

where the positive numbers b_K will be chosen later. It is positive semi-definite, supported by a graph, yet it is not divergence-free, since $\mathrm{Div}\, T' = \sum b_K \mathrm{Div}\, S_K \neq 0$. Because $\mathrm{Div}\, S_K$ is a sum of Dirac masses at the end points $x^* \pm \varepsilon z_j$, we have instead

$$\|\mathrm{Div}\, T'\| = 2(n-1) \sum_{\text{kinks in } H_\tau} b_K.$$

At initial and final time, T' coincides with T, and therefore we have

$$\|T'_{0\bullet}(t=0)\| = m \sum \sqrt{1 + |v(0)|^2}$$

where the sum runs over the particles. We infer

$$\|T'_{0\bullet}(t=0)\| \leq m \sum \left(1 + \frac{|v(0)|^2}{2}\right) \leq M + E.$$

Likewise we also have $\|T'_{0\bullet}(t=\tau)\| \leq M + E$. Since T' is a finite measure, we are therefore in position to apply Compensated Integrability to T' in H_τ.

Now the left-hand side of (17) involves the integral of $(\det T')^{\frac{1}{n}}$, which vanishes identically, and the determinantal masses at the kinks of the trajectories. A kink K at a point x^* involve the three vectors mV, mV' and $Q = -m(V + V')$. A combination of Corollaries 4.1, 4.2 and of formula (23) yields the following calculation (here we have $p = 2$ and $q = n-1$):

$$\mathrm{Dm}(T'; x^*) = 2^{n-3} b_K^{\frac{n-1}{n}} m^{\frac{2}{n}} |V \wedge V'|^{\frac{1}{n}}$$

Writing (17) for the tensor T', we obtain

$$\sum_{\text{kinks in } H_\tau} b_K^{\frac{n-1}{n}} m^{\frac{2}{n}} |V \wedge V'|^{\frac{1}{n}} \leq c_n \left(2(M+E) + 2(n-1) \sum_{\text{kinks in } H_\tau} b_K \right)^{1+\frac{1}{n}}$$

for another universal constant, still denoted c_n.

We now introduce auxiliary parameters $\lambda > 0$ and $\beta_K > 0$, and we set $b_K = \lambda \beta_K^{\frac{n}{n-1}}$. We infer

$$\sum_{\text{kinks in } H_\tau} \beta_K m^{\frac{2}{n}} |V \wedge V'|^{\frac{1}{n}} \leq c_n \lambda^{\frac{1}{n}-1} \left(M+E+\lambda(n-1) \sum_{\text{kinks in } H_\tau} \beta_K^{\frac{n}{n-1}} \right)^{1+\frac{1}{n}}.$$

Choosing

$$\lambda := (M+E) \left(\sum_{\text{kinks in } H_\tau} \beta_K^{\frac{n}{n-1}} \right)^{-1},$$

we infer

$$\sum_{\text{kinks in } H_\tau} \beta_K m^{\frac{2}{n}} |V \wedge V'|^{\frac{1}{n}} \leq c_n (M+E)^{\frac{2}{n}} \|\vec{\beta}\|_{\ell^{\frac{n}{n-1}}}.$$

The above inequality is valid for every choice of positive parameters β_K. Since the left-hand side is a scalar product $\langle \vec{\beta}, \vec{D} \rangle$, and since the dual space of $\ell^{\frac{n}{n-1}}$ is ℓ^n, it tells us that

$$\|\vec{D}\|_{\ell^n} \leq c_n (M+E)^{\frac{2}{n}}.$$

In other words, we have

$$m^2 \sum_{\text{kinks in } H_\tau} |V \wedge V'| \leq c_n (M+E)^2.$$

Since

$$|V \wedge V'| = \sqrt{|v'-v|^2 + |v \wedge v'|^2},$$

we obtain our first estimate

$$m^2 \sum_{\text{kinks in } H_\tau} \sqrt{|v'-v|^2 + |v \wedge v'|^2} \leq c_n (M+E)^2.$$

Remarking that the right-hand side does not depend upon the time length τ, we actually have

$$m^2 \sum_{\text{kinks in } H_\infty} \sqrt{|v'-v|^2 + |v \wedge v'|^2} \leq c_n (M+E)^2, \tag{24}$$

where now the sum extends over all the history.

Using the scaling. Equation (24) is not acceptable from a physical point of view. It lacks homogeneity: One should not add a mass and an energy (right-hand side) or two different powers of velocities (left-hand side). To overcome this flaw, we notice that from a given flow, one can construct a one-parameter family of flows, by changing the time scale. This trick was used already in the context of the Euler equations of a compressible fluid, see [12].

We consider particles of same radius a. If $\mu > 0$ is given, a trajectory $t \mapsto X(t)$ in the original flow $\mathcal{F}_1$ gives rise to a trajectory $t \mapsto X_\mu(t) := X(\mu t)$ in the new flow $\mathcal{F}_\mu$. The velocity is $v_\mu(t) = \mu v(\mu t)$. The flow parameters become

$$M_\mu = M, \qquad E_\mu = \mu^2 E, \qquad \bar{v}_\mu = \mu \bar{v}.$$

Applying (24) to $\mathcal{F}_\mu$ results in a parametrized inequality

$$m^2 \sum_{\text{kinks in } H_\infty} \sqrt{\mu^2 |v' - v|^2 + \mu^4 |v \wedge v'|^2} \leq c_n (M + \mu^2 E)^2, \qquad \forall \mu > 0.$$

Choosing $\mu^2 = M/2E = \bar{v}^{-2}$, we obtain

$$m^2 \sum_{\text{kinks in } H_\infty} \sqrt{\bar{v}^2 |v' - v|^2 + |v \wedge v'|^2} \leq c_n M^2 \bar{v}^2.$$

This is equivalent to (7) because of

$$\frac{a+b}{2} \leq \sqrt{a^2 + b^2} \leq a + b$$

for positive numbers. This ends the proof of Theorem 1.1.

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