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A derivation of the Liouville equation for hard particle dynamics with non-conservative interactions

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The Liouville equation is of fundamental importance in the derivation of continuum models for physical systems which are approximated by interacting particles. However, when particles undergo instantaneous interactions such as collisions, the derivation of the Liouville equation must be adapted to exclude non-physical particle positions, and include the effect of instantaneous interactions. We present the weak formulation of the Liouville equation for interacting particles with general particle dynamics and interactions, and discuss the results using two examples.

Keywords: Liouville equation; Hard particles; BBGKY hierarchy; Inelastic collisions

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1. Introduction

Many physical systems can be modelled as a collection of interacting particles, for example, interactions in and between molecules [18], colloidal systems [9] or systems of granular media [3, 12, 15]. However, when considering a large number of particles, simulating such a system as a discrete set of particles quickly becomes computationally intractable. In these cases, it is necessary to consider a continuous approximation of the system. One of the most popular first steps to a valid continuous model is the Liouville equation (when particle dynamics are deterministic) or the Kramers equation (when particle dynamics are stochastic) [16].

We assume that a system of N particles in d dimensions with positions $X(t) \in \mathbb{R}^{dN}$ and velocities $V(t) \in \mathbb{R}^{dN}$ at time $t \in \mathbb{R}$ is governed by Newton's equations:

$$\frac{\mathrm{d}X(t)}{\mathrm{d}t} = \frac{V(t)}{m}, \quad \frac{\mathrm{d}V(t)}{\mathrm{d}t} = G(X(t), V(t), t), \tag{1.1}$$

where $G(X, V, t)$ incorporates external effects such as gravity and friction, and inter-particle interactions such as cohesion in granular media or intermolecular forces in molecular dynamics. Under the assumption that the microscopic dynamics are smooth, associated with the microscopic dynamics is the Liouville equation, a partial differential equation which determines the dynamics of the N-body distribution function $f^{(N)}$, which is *formally* given by

$$\mathcal{M}[f^{(N)}] := \left[\frac{\partial}{\partial t} + \frac{1}{m} v \cdot \nabla_X - \nabla_V \cdot G(X, V, t)\right] f^{(N)}(X, V, t) = 0. \tag{1.2}$$

For point-like particles and sufficiently-smooth G, equation (1.2) fully describes the evolution of an initial configuration of particles $f_0^{(N)}$. However, when particles are of finite volume, adjustments have to be made to the microscopic dynamics to avoid non-physical particle overlap. Under the assumption that particles are spherical and of radius $\varepsilon > 0$, and that interaction is through pairwise collisions, a binary collision rule can be introduced that instantaneously changes the velocities of two particles so that they are moving away from each other immediately after contact. Indeed, if at time t particles i and j have positions x_i, x_j and velocities $v_i^{\text{in}}, v_j^{\text{in}}$, respectively, such that $(v_i^{\text{in}} - v_j^{\text{in}}) \cdot (x_i - x_j) < 0$ and $\|x_i - x_j\| = \varepsilon$, under the assumption that collisions are elastic (i.e. no energy is lost due to the collision) velocities are updated using the following rules:

$$\begin{aligned} v_i^{\text{out}} &= v_i^{\text{in}} - \frac{x_i - x_j}{\|x_i - x_j\|} \cdot (v_i^{\text{in}} - v_j^{\text{in}}) \frac{x_i - x_j}{\|x_i - x_j\|}, \\ v_j^{\text{out}} &= v_j^{\text{in}} + \frac{x_i - x_j}{\|x_i - x_j\|} \cdot (v_i^{\text{in}} - v_j^{\text{in}}) \frac{x_i - x_j}{\|x_i - x_j\|}. \end{aligned} \tag{1.3}$$

Notably the velocity components in the direction of $x_i - x_j$ are swapped and reflected.

At an informal level, the collisional effect is not recognized at the level of the Liouville equation, but is derived in the Bogoliubov–Born–Green–Kirkwood–Yvon (BBGKY) hierarchy [**1**, **19**], for example, as a consequence of additional assumptions on an interaction force [**10**]. However, by instantaneously changing the velocities of two particles that undergo a collision, a fundamental assumption in the Liouville derivation is no longer valid—the dynamics of an individual particle are no longer smooth. We therefore cannot rely on the correctness of the statement of the Liouville equation in equation (1.2) above, and must resort to an alternative formulation to derive an equation for $f^{(N)}(X, V, t)$. A suitable alternative is the *weak formulation* of the Liouville equation [**20**].

In a paper of the third author [**20**], a system of $N = 2$ spherical particles with diameter $\varepsilon > 0$ and $G(X, V, t) = 0$ is fully characterized, and, under no additional assumptions, it is shown that for all smooth, compactly supported test functions Φ, given initial data $f_0^{(2)} \in C^0(\mathcal{D}) \cap L^1(\mathcal{D})$ (i.e. the space of all continuous functions with compact support), such that $f_0^{(2)}$ integrates to 1 on the phase space, and is always positive, there exists a unique $f^{(2)} \in C^0((-\infty, \infty), L^1(\mathcal{D}))$ which satisfies the weak formulation

$$\int_{\mathcal{P}_\varepsilon}\int_{\mathbb{R}^6}\int_{-\infty}^{\infty}\left[\frac{\partial\Phi(X,V,t)}{\partial t}+(V\cdot\nabla_X)\Phi(X,V,t)\right]f^{(2)}(X,V,t)\,\mathrm{d}t\,\mathrm{d}V\,\mathrm{d}X$$
$$=$$
$$-\int_{\partial\mathcal{P}_\varepsilon}\int_{\mathbb{R}^6}\int_{-\infty}^{\infty}\Phi(X,V,t)f^{(2)}(X,V,t)V\cdot\hat{\nu}(X)\,\mathrm{d}t\,\mathrm{d}V\,\mathrm{d}\mathcal{H}(X) \qquad (1.4)$$

for all test functions Φ, and which conserves linear and angular momentum, and kinetic energy. In the above:

- we define the spatial integral on $\mathcal{P}_\varepsilon := \{X \in \mathbb{R}^6 : \|x_1 - x_2\| \geqslant \varepsilon\}$, as particles cannot overlap;
- $\mathcal{D} \in \mathbb{R}^{12}$ represents all possible configurations of positions and velocities, given that two particles cannot overlap ($X \in \mathcal{P}_\varepsilon$);
- the vector $\hat{\nu} \in \mathbb{R}^6$ is the outward unit normal to the surface $\partial\mathcal{P}$;
- $\mathcal{H}$ is the Hausdorff measure [**6**] on $\partial\mathcal{P}_\varepsilon$.

In this case, we say that $f^{(2)}$ is a global-in-time weak solution of the Liouville equation given by

$$\frac{\partial f^{(2)}}{\partial t}+(V\cdot\nabla_X)f^{(2)}=\mathcal{B}_X[f^{(2)}], \qquad (1.5)$$

where $\mathcal{B}_X[f^{(2)}]$ is determined in the weak sense against all differentiable, compactly supported test functions $\Phi \in C_c^1((-\infty,\infty),\mathcal{D})$:

$$\langle\mathcal{B}_X[f^{(2)}],\Phi\rangle=\int_{\partial\mathcal{P}_\varepsilon}\int_{\mathbb{R}^6}f^{(2)}(X,V,t)\Phi(X,V,t)V\cdot\hat{\eta}_Y\,\mathrm{d}V\,\mathrm{d}\mathcal{H}(Y). \qquad (1.6)$$

In contrast to classical formulations [**11**], a collisional term $\mathcal{B}_X[f^{(2)}]$ is derived at the level of the Liouville equation. Furthermore, under the assumptions of molecular chaos, $\mathcal{B}_X[f^{(2)}]$ admits the elastic Boltzmann collision operator [**4**, **7**] in the first equation of the weak formulation of the BBGKY hierarchy, agreeing with previous results. Under restrictions on initial data, for example, on the particle density of the system, an analogue to equation (1.5) should also hold in systems with more than 2 particles.

From this point, a clear question to consider is how more complicated dynamics, or other instantaneous interactions between particles, affect the derivation of equation (1.5). In this paper, we derive the weak formulation of the Liouville equation for two particles with general free dynamics (i.e. where there are no instantaneous interactions between particles), and general instantaneous interactions (i.e. general collisional events and events where particles are refracted away from one another). The microscopic dynamics are first discussed in § 2, which leads to the derivation of the Liouville equation in § 3. This careful examination of the dynamics provides useful insights for mathematical modelling of materials approximated by

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hard particles, e.g. granular media. In particular, the collision operators (in both position and velocity) constructed at the level of the Liouville equation in the weak formulation should be of interest.

Following this, we consider an example in § 4 where collisions are *inelastic* and the free dynamics are affected by external friction and a constant external potential. Upon consideration of the weak Liouville equation, and the admissible initial data for the given dynamics, this example leads to a modified collisional term at the level of the BBGKY hierarchy. We provide a further example which displays our results in equation (5), where we consider a system of particles where the free dynamics are linear, but particles interact via a discrete *square-shoulder* interaction potential, equation (5.1). The inclusion of this discrete potential then leads to an additional collision term in the Liouville equation, which translates to a truncated Boltzmann collision operator in the BBGKY hierarchy. We discuss our findings and future directions for research in § 6.

1.1. Set-up

1.1.1. *Free particle dynamics* At the microscopic level, we consider the initial data of two particles. The first particle has initial position $x \in \mathbb{R}^3$ and velocity $v \in \mathbb{R}^3$, the second has initial position $\bar{x} \in \mathbb{R}^3$ and velocity $\bar{v} \in \mathbb{R}^3$, all assumed at time $t = 0$. When considering the initial position of particles, we refer to the position of their centres of mass. It is useful to consider the concatenation of position and velocities as $X = [x, \bar{x}] \in \mathbb{R}^6$ and $V = [v, \bar{v}] \in \mathbb{R}^6$. In some cases it is useful to define $Z = [X, V] \in \mathbb{R}^{12}$ in the same spirit.

One of the important requirements of our method is an understanding of admissible initial data, i.e. initial data that produces a solution to equation (1.1) for all time $t \in \mathbb{R}$. In this paper, we assume that the admissible initial position data for the free dynamics (i.e. for point-like particles) encompasses the entirety of $\mathbb{R}^6$, i.e. any initial positions can provide dynamics that are defined for all times $t \in \mathbb{R}$. However, the initial position data $X \in \mathbb{R}^6$ may restrict the admissible initial velocity data to a subset of $\mathbb{R}^6$. Therefore, for each $X \in \mathbb{R}^6$, we define $\mathcal{V}^{\mathrm{f}}(X) \subseteq \mathbb{R}^6$ to be the set of initial velocity data which produces a solution to equation (1.1) for all times $t \in \mathbb{R}$, and take $V \in \mathcal{V}^{\mathrm{f}}(X)$.

Many calculations in this derivation refer to relative differences of position and velocity of the two particles, for example, the binary collision rule equation (1.3) is used in the dynamics when $(x - \bar{x}) \cdot (v - \bar{v}) < 0$. Thus we introduce the following notation: for a vector $A = [a, \bar{a}] \in \mathbb{R}^6$, we write $\tilde{a} = a - \bar{a} \in \mathbb{R}^3$ as its relative difference. Much of the intuition in the derivation can be considered in terms of relative differences of particle data. For example, we can rewrite the dynamics of the pair of particles in terms of relative differences, which effectively fixes one point at position 0 with radius ε, and a collision is seen as a reflection of an intersecting point-particle trajectory.

Given initial data $X \in \mathbb{R}^6$ and $V \in \mathcal{V}^{\mathrm{f}}(X)$, we define the free particle flow maps for position and velocity by $\Phi_t^x(X, V)$ and $\Phi_t^v(X, V)$, respectively, and assume that they satisfy the Newton equations of motion, namely

$$\partial_t \Phi_t^x(X, V, t) = \Phi_t^v(X, V, t), \quad \partial_t \Phi_t^v(X, V, t) = G(\Phi_t^x(X, V, t), \Phi_t^v(X, V, t), t). \quad (1.7)$$

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We write $\Phi_t = [\Phi_t^x, \Phi_t^v]$ as the flow map defined on initial data $Z \in \mathcal{D}$ for all times $t \in \mathbb{R}$. We also assume that the flow maps produce unique trajectories for any given initial data.

1.1.2. *Dynamics with instantaneous interactions* When instantaneous interactions are considered, a careful understanding of the admissible data is required. Outside of the discrete set of interaction times the particles follow trajectories determined by Φ_t^x and Φ_t^v. In this section, we will construct the flow maps Ψ_t^x and Ψ_t^v that include instantaneous interactions.

Admissible Data. In both of the examples we consider, the particles are hard spheres with diameter ε. The possible initial data for X is therefore restricted to the *hard sphere table*

$$\mathcal{P}_\varepsilon = \{X = [x, \bar{x}] \in \mathbb{R}^6 : \|x - \bar{x}\| \geqslant \varepsilon\}. \tag{1.8}$$

The subset $\mathcal{P}_\varepsilon \subseteq \mathbb{R}^6$ is a real analytic manifold with boundary $\partial\mathcal{P}_\varepsilon$, which has outward unit norm vector

$$\hat{\nu} = \frac{1}{\sqrt{2}\varepsilon}[-\tilde{x}, \tilde{x}] \tag{1.9}$$

for $X \in \partial\mathcal{P}_\varepsilon$.

We assume that the motion of the spherical particles is non-rotational, i.e. we do not furnish the equations of motion with an evolution equation for the angular velocity of the spheres. Adopting the assumption of smooth spherical particles is very popular in the literature, whilst the introduction of particles which are non-spherical is also of interest and has been studied, for example, computationally in [5].

The introduction of instantaneous interactions between particles will change which initial velocities are admissible. We define the set of admissible velocity data for dynamics with instantaneous interactions as $\mathcal{V}(X)$ for each $X \in \mathcal{P}_\varepsilon$, which we assume has a piecewise analytic boundary. Furthermore, we define $\mathcal{C}(X) \subset \mathcal{V}(X)$ to be the set of initial data which leads to instantaneous interactions, and also assume that $\partial\mathcal{C}(X)$ is a piecewise analytic submanifold of $\mathbb{R}^6$. We validate this in the two examples considered.

We may consider additional interaction diameters $\mathcal{P}_{\tilde{\varepsilon}}$ for $\tilde{\varepsilon} > \varepsilon$, e.g. square well interactions discussed in [2], but importantly for $X \in \mathbb{R}^6 \backslash \mathcal{P}_\varepsilon$, $\mathcal{V}(X) = \emptyset$. We define the set of interaction diameters by $\Theta = \{\varepsilon_i \in \mathbb{R}^+, i = 1, \ldots, m : \varepsilon_m > \varepsilon_{m-1} > \cdots > \varepsilon_0 > 0\}$ where m is the number of interaction diameters of an individual particle.

We assume that the dynamics with instantaneous interactions have flow maps $\Psi_t^x(X, V)$ and $\Psi_t^v(X, V)$, which are defined globally in time.

Event Times. We will characterize each instantaneous event by an event time, an interaction diameter and an event map that changes the particle velocities. As interactions are instantaneous, the event times can be enumerated as a discrete set, which can be finite or infinite. We write the event times as $\tau_i \in \mathbb{R}$ for $i = -M, -M + 1, \ldots, -1, 0, 1, \ldots, N-1, N$, where $M = M(X, V), N = N(X, V) \in \mathbb{N} \cup \{\infty\}$, and

$$-\infty = \tau_{-M}(X, V) < \tau_{-M+1}(X, V) < \cdots < \tau_{N-1}(X, V) < \tau_N(X, V) = \infty, \tag{1.10}$$

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where we choose τ_0 to be the closest event time to time $t = 0$:

$$\tau_0 = \arg\min_{|s|}\{s \in \mathbb{R} : \tilde{\Phi}_s(X, V) \in \partial\mathcal{P}_{\bar{\varepsilon}}, \bar{\varepsilon} \in \Theta\}. \tag{1.11}$$

In turn each τ_i can be defined in terms of the previous or next event time. When the previous event time has been defined:

$$\tau_{i+1}(X, V) := \arg\min_{|s|}\{s \in (\tau_i, \infty) : \Phi_{s-\tau_i}(\Psi^x_{\tau_i}, \Psi^v_{\tau_i}) \in \partial\mathcal{P}_{\bar{\varepsilon}}, \bar{\varepsilon} \in \Theta\}, \tag{1.12}$$

and when the next event has been defined:

$$\tau_{i-1}(X, V) := \arg\min_{|s|}\{s \in (-\infty, \tau_i) : \Phi_{s-\tau_i}(\Psi^x_{\tau_i}, \Psi^v_{\tau_i}) \in \partial\mathcal{P}_{\bar{\varepsilon}}, \bar{\varepsilon} \in \Theta\}. \tag{1.13}$$

Events occur when particles reach an interaction diameter. We will assume that there exists $\delta > 0$ such that for all $i = -M, \ldots, N$, $\tau_i - \tau_{i-1} > \delta$, and we define two special event times, namely $\tau_{-M}(X, V) = -\infty$, $\tau_N(X, V) = \infty$. Between each pair of event times, the particle dynamics are determined by equation (1.1). At each time τ_i, the particles experience an instantaneous change in velocity. For hard spheres, for example, this will ensure that the two particles do not overlap.

Event Maps. At each time τ_i, the velocities of the particles experience an instantaneous change. By the formal axioms of classical mechanics, it is necessary for the change in velocities to conserve linear and angular momentum, i.e. if an event $\tau_i(X, V), X \in \mathcal{P}_\varepsilon, V \in \mathcal{V}(X)$ occurs at time $t = 0$ (without loss of generality), then

$$v' + \bar{v}' = v + \bar{v}, \tag{1.14}$$

and for all $a \in \mathbb{R}^3$,

$$(x - a) \times v' + (\bar{x} - a) \times \bar{v}' = (x - a) \times v + (\bar{x} - a) \times \bar{v}, \tag{1.15}$$

where primed velocities denote post event velocities. In fact, to show conservation of angular momentum one only needs to check equation (1.15) is satisfied for 4 values of a.

Proposition 1.1. *Equations* (1.15) *and* (1.14) *are true for all* $a \in \mathbb{R}^3$ *if and only if*

$$(x - p_i) \times v' + (\bar{x} - p_i) \times \bar{v}' = (x - p_i) \times v + (\bar{x} - p_i) \times \bar{v}, \tag{1.16}$$

for $i = 1, \ldots, 4$, *where* $\{p_i\}_{i=1}^4 \subset \mathbb{R}^3$ *are the vertices of a (non-degenerate) polytope in* $\mathbb{R}^3$.

Proof. The necessity of this statement is trivial. For sufficiency, by equation (1.14) we may assume $x = 0$ without loss of generality, and so for each p_j, for all constants

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$c_j \in \mathbb{R}$, we have

$$
\begin{aligned}
& -c_j p_j \times v' + c_j(\bar{x} - p_j) \times \bar{v}' = -c_j p_j \times v + c_j(\bar{x} - p_j) \times \bar{v} \\
\implies & -\sum_{j=1}^{4} c_j p_j \times v' + \sum_{j=1}^{4} c_j(\bar{x} - p_j) \times \bar{v}' = -\sum_{j=1}^{4} c_j p_j \times v + \sum_{j=1}^{4} c_j(\bar{x} - p_j) \times \bar{v}.
\end{aligned}
$$

If we now suppose that $\sum_{j=1}^{4} c_j = 1$, then we have that equation (1.15) is satisfied for all q in the set

$$
\mathcal{C} = \left\{ \sum_{i=1}^{4} c_j p_j : \sum_{j=1}^{4} c_j = 1 \right\}. \tag{1.17}
$$

As $\mathcal{C}$ is a convex set in $\mathbb{R}^3$, we infer that $\mathcal{C} = \mathbb{R}^3$, as required. □

Considering the 'concatenation' notation, the change in velocity is determined by a map $\sigma_i : \mathbb{R}^6 \to \mathbb{R}^6$, where $\sigma_i(X, V) \in \mathbb{R}^{6\times 6}$. We have the following result on the form of $\sigma(X, V)$.

THEOREM 1.2. *Let $X \in \mathbb{R}^6$ and $V \in \mathbb{R}^6$, and set $X = [x, \bar{x}], V = [v, \bar{v}]$. Assume that $\bar{x} \neq x$, and set*

$$
N(X) = \frac{1}{\|x - \bar{x}\|}[x - \bar{x}, \bar{x} - x]. \tag{1.18}
$$

Then the following are equivalent:

(i)

$$
\sigma(X, V) = I + \eta(X, V) N(X) \otimes N(X), \tag{1.19}
$$

for some $\eta : \mathbb{R}^{12} \to \mathbb{R}$.

(ii) *The map σ respects the conservation of total linear and angular momentum:*

(a) *(COLM)*

$$
v' + \bar{v}' = v + \bar{v}; \tag{1.20}
$$

(b) *(COAM) For any $a \in \mathbb{R}^3$,*

$$
(x - a) \times v' + (\bar{x} - a) \times \bar{v}', = (x - a) \times v + (\bar{x} - a) \times \bar{v}, \tag{1.21}
$$

where $v' = (\sigma(X, V)V)_{(1,2,3)}$, and $\bar{v}' = (\sigma(X, V)V)_{(4,5,6)}$[1].

[1]i.e. the effect of $\sigma(X, V)$ on the first and last three entries of V respectively.

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Proof. We note that equation (1.21) can be written as $A\sigma(X,V)V = AV$, where

$$A_a = \begin{pmatrix} 0 & -x_3^a & x_2^a & 0 & -\bar{x}_3^a & \bar{x}_2 \\ x_3^a & 0 & -x_1^a & \bar{x}_3^a & 0 & -\bar{x}_1^a \\ -x_2^a & x_1^a & 0 & -\bar{x}_2^a & \bar{x}_1^a & 0 \end{pmatrix}, \tag{1.22}$$

where we have written $x_i^a = x_i - a$. One can show that ($1 \implies 2$) by a direct calculation. We see that

$$\begin{aligned} A + a\sigma(X,V) &= A_a(I - \eta(X,V)N \otimes N), \\ &= A_a - \eta(X,V)A_a N(X) \otimes N(X) = A_a, \end{aligned}$$

where it holds that $A_a N(X) = (0,0,0)$. With a view to demonstrating that ($2 \implies 1$), we note that the matrix A_a is rank 3 (by considering its row-echelon form), and that it is enough to show that equation (1.21) holds for $a = \{a_1, a_2, a_3, a_4\}$, if equation (1.20) holds.

We note that $A_a\sigma(X,V)V = A_a V$ for all $V \in \mathbb{R}^6$ implies that $A_a(\sigma(X,V)V - V) = 0$. Therefore, $\sigma(X,V)V - V \in \ker(A_a)$ for all $a \in \mathbb{R}^6$. Let $Y = (\sigma(X,V)V - V)$; then

$$-Y_2 x_3^a + Y_3 x_2^a - Y_5 \bar{x}_3^a + Y_6 \bar{x}_2^a = 0, \quad Y_1 x_3^a - Y_3 x_1^a + Y_4 \bar{x}_3^a - Y_6 \bar{x}_1^a = 0,$$
$$-Y_1 x_2^a + Y_2 x_1^a - Y_4 \bar{x}_2^a + Y_5 \bar{x}_1^a = 0.$$

We consider the values of observation vectors given by

$$a_1 = (x_1, x_2, x_3), \quad a_2 = (x_1, x_2, \bar{x}_3),$$
$$a_3 = (x_1, \bar{x}_2, \bar{x}_3), \quad a_4 = (\bar{x}_1, \bar{x}_2, \bar{x}_3),$$

which form the four vertices of a tetrahedron, which results in

$$Y = \tilde{\eta}(x,v) \begin{pmatrix} x_1 - \bar{x}_1 \\ x_2 - \bar{x}_2 \\ x_3 - \bar{x}_3 \\ \bar{x}_1 - x_1 \\ \bar{x}_2 - x_2 \\ \bar{x}_3 - x_3 \end{pmatrix} = \eta(X,V)N(X), \tag{1.23}$$

where $\eta(X,V) = \|x - \bar{x}\|\tilde{\eta}(X,V)$. We note, taking dot products on both sides of equation (1.23) with $N(X)$ and rearranging, that

$$\begin{aligned} & N(X) \cdot (\sigma(X,V) - V) = \eta(X) \\ \implies & (I - N(X) \otimes N(X))\sigma(X,V)V = (I - N(X) \otimes N(X))V, \end{aligned}$$

i.e. σ can only change the component of V in the direction of $N(X)$. Thus, if $N(X) \cdot V = 0$, then V is contained in the hyperplane orthogonal to $N(X)$, and we must have that $\sigma(X,V)V = V$. Therefore, without loss of generality, for any $V \in \mathbb{R}^6$ we can take $\eta(X,V) = N(X) \cdot V\tilde{\eta}(X,V)$, and so

$$\sigma(X,V)V = (I + \eta(X,V)N(X) \otimes N(X))V \tag{1.24}$$

as claimed. □

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Equations (1.14), (1.15) are not enough to fully determine the map σ; an additional constraint must be supplied. For example, in [20], it is shown that the Boltzmann (elastic) scattering map can be determined by including the conservation of kinetic energy. In this case σ is an involution, i.e. $\sigma(X,V)^2 = I$. Alternative maps can be derived using different constraints on the Jacobian of the scattering map (for inelastic Boltzmann scattering maps considered in § 4), or on kinetic energy (for boost or damping maps considered in [2]). We call this the *event map constraint*.

We define the forward time map σ_i^+ as the map which takes pre-event velocities to post-event velocities, and the backward time map σ_i^- taking post-event velocities to pre-event velocities. For the dynamics to be reversible we require $\sigma_i^+(X,V)\sigma_i^-(X,V) = I$. Note that if we assume that $\sigma_i^-(X,V) = \sigma_i^+(X,V)$ then $\eta(X,V) = 0$ or $\eta(X,V) = -2$. The former value of $\eta(X,V)$ produces the identity map, while the latter is the elastic Boltzmann scattering map.

We can fully define the flow maps for dynamics with instantaneous interactions, using $\Phi_t^x, \Phi_t^v, \tau_i$ and $\sigma_i^{\pm}$. We split the initial data into two cases.

No Instantaneous Events. If X, V are such that no instantaneous events happen, then $M + N = 1$ and Ψ_t^X, Ψ_t^v obey

$$\partial_t \Psi_t^x(X,V) = \Phi_t^x(X,V), \quad \partial_t \Psi_t^v(X,V) = G(X,V,t) \tag{1.25}$$

in the classical sense.

Instantaneous Events. When X, V are such that instantaneous events occur in finite time, then

$$\partial_t \Psi_t^x(X,V) = \begin{cases} \Phi_t^v(X,V), & \tau_{i_0-1} \leqslant t \leqslant \tau_{i_0}, \\ \Phi_{t-\tau_i}^v(\Psi_{\tau_i}^x(X,V), \sigma_i^+ \Psi_{\tau_i}^v(X,V)), & \tau_i < t \leqslant \tau_{i+1}, \\ & i = i_0, \dots, N-1, \\ \Phi_{t-\tau_i}^v(\Psi_{\tau_i}^x(X,V), \sigma_i^- \Psi_{\tau_i}^v(X,V)), & \tau_{i-1} \leqslant t < \tau_i, \\ & i = -(M+1), \dots, (i_0 - 1), \end{cases} \tag{1.26}$$

and

$$\partial_t \Psi_t^v(X,V) = \begin{cases} G(X,V,t), & \tau_{i_0-1} \leqslant t \leqslant \tau_{i_0}, \\ G(\Psi_{\tau_i}^x(X,V), \sigma_i^+ \Psi_{\tau_i}^v(X,V), t-\tau_i), & \tau_i < t \leqslant \tau_{i+1}, \\ & i = i_0, \dots, N-1, \\ G(\Psi_{\tau_i}^x(X,V), \sigma_i^- \Psi_{\tau_i}^v(X,V), t-\tau_i), & \tau_{i-1} \leqslant t < \tau_i, \\ & i = -(M+1), \dots, (i_0 - 1), \end{cases} \tag{1.27}$$

where $i_0 = 1$ if $\tau_0 < 0$ and $\mu = 0$ if $\tau_0 > 0$.

Note that free particle flow maps need not be defined globally to be used in these flow maps, if the instantaneous interaction renders the trajectory admissible.

We now have all the necessary notation to state the main results of this paper.

1.2. Main results

Now that we have fully defined the dynamics of two particles, we are in a position to state the main results of this paper. To do so, we state the following definition, which is generalized from [20].

DEFINITION 1.3 (*Global in time weak solutions of the Liouville equation*). Suppose we are given an initial condition $f_0 \in C^0(\mathcal{D}) \cap L^1(\mathcal{D})$, such that

$$\int_{\mathcal{P}_\varepsilon} \int_{\mathcal{V}(X)} f_0(X,V)\,\mathrm{d}V\,\mathrm{d}X = 1, \quad f_0(X,V) \geqslant 0. \tag{1.28}$$

Then $f \in C^0((-\infty,\infty), L^1(\mathcal{D}))$ is a physical global in time solution of the Liouville equation

$$\partial_t f + V\cdot\nabla_X f + \nabla_V\cdot(G(X,V,t)f) = \mathcal{B}_X[f^{(2)}] + \mathcal{B}_V[f^{(2)}] \tag{1.29}$$

if and only if for all test functions $\Phi \in C_c^1(T\mathbb{R}^6 \times (-\infty,\infty))$ with spatial support in $\mathcal{P}_\varepsilon$, it holds that

$$\begin{aligned}
&\int_{\mathcal{P}_\varepsilon}\int_{\mathcal{V}(X)}\int_{-\infty}^{\infty} f(X,V,t)[\partial_t\Phi(X,V,t) + V\cdot\nabla_X\Phi(X,V,t)\\
&\qquad + \nabla_V\cdot(G(X,V,t)\Phi(X,V,t))]\,\mathrm{d}t\,\mathrm{d}V\,\mathrm{d}X\\
&=\\
&-\int_{\partial\mathcal{P}_\varepsilon}\int_{\mathcal{V}(X)}\int_{-\infty}^{\infty} f(X,V,t)\Phi(X,V,t)V\cdot\hat{\nu}_X\,\mathrm{d}t\,\mathrm{d}V\,\mathrm{d}\mathcal{H}(X)\\
&-\int_{\mathcal{P}_\varepsilon}\int_{\partial\mathcal{V}(X)}\int_{-\infty}^{\infty} f(X,V,t)\Phi(X,V,t)G(X,V,t)\cdot\hat{\nu}_V\,\mathrm{d}t\,\mathrm{d}\mathcal{H}(X,V)\,\mathrm{d}X,
\end{aligned} \tag{1.30}$$

and f obeys the conservation of linear and angular momentum for all $t \in (-\infty,\infty)$:

$$\int_{\mathcal{P}_\varepsilon}\int_{\mathcal{V}(X)} (v+\bar{v})f(X,V,t)\,\mathrm{d}V\,\mathrm{d}x = \int_{\mathcal{P}_\varepsilon}\int_{\mathcal{V}(X)} (v+\bar{v})f_0(X,V)\,\mathrm{d}V\,\mathrm{d}x, \tag{1.31}$$

$$\int_{\mathcal{P}_\varepsilon}\int_{\mathcal{V}(X)} (x\times v+\bar{x}\times\bar{v})f(X,V,t)\,\mathrm{d}V\,\mathrm{d}x = \int_{\mathcal{P}_\varepsilon}\int_{\mathcal{V}(X)} (x\times v+\bar{x}\times\bar{v})f_0(X,V)\,\mathrm{d}V\,\mathrm{d}x, \tag{1.32}$$

and the microscopic dynamics satisfy the associated event map constraints.

With this, we state the main result of this paper.

THEOREM 1.4 Existence of global-in-time weak solutions of the Liouville equation. *For any $f_0 \in C^0(\mathcal{D}) \cap L^1(\mathcal{D})$, there exists a physical global-in-time weak solution of the Liouville equation* (1.30).

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Before identifying important transport identities and proving theorem 1.4, we make some remarks on this result.

Firstly, we have made very few assumptions on the free dynamics of the particles; they can be affected by external or interparticle forces. In § 4 we consider inelastic collisions, but the same formulation can be used to consider any interactions determined by discrete step potentials [**2**]. Our result is therefore quite general, and should be appropriate for a range of systems.

The Liouville equation is derived for a system of two particles. In principle, systems of many particles may involve many body interactions. However, given the correct subset of initial data, which ensures that all instantaneous interactions are pairwise, the equation (1.30) should also be accurate for systems of many particles, and may be used to approximate systems where the initial data is not so carefully constructed.

We can also state a general form of the BBGKY hierarchy. We start with a definition of global in time weak solutions thereof.

Definition 1.5. Let $f_0 \in C^1(\mathcal{D}) \cap L^1(\mathcal{D})$ be symmetric in its particle arguments (*i.e.* $[v, x]$ and $[\bar{v}, \bar{x}]$ can be interchanged, leaving its value unchanged). We say that a pair of maps $(f_0^{(1)}, f_0^{(2)})$ with membership

$$f^{(1)} \in C^0((-\infty,\infty), L^1(T\mathbb{R}^3)), \quad f^{(2)} \in C^0((-\infty,\infty), L^2(\mathcal{D})) \tag{1.33}$$

is a global in time weak solution of the BBGKY hierarchy associated to the initial data

$$f_0^{(1)} = \int_{\mathbb{R}^3 \setminus B_\varepsilon(x)} \int_{\mathcal{V}(x,\bar{x},v)} f_0(X,V)\, \mathrm{d}\bar{v}\, \mathrm{d}\bar{x} \text{ for all } [x, v] \in T\mathbb{R}^3, \tag{1.34}$$

where $B_\varepsilon(x) \subset \mathbb{R}^3$ is the ball of radius ε centred at x, and

$$f_0^{(2)}(X,V) = f_0(X,V) \text{ for all } [X,V] \in \mathcal{D}, \tag{1.35}$$

if and only if, for all test functions $\phi \in C_c^\infty(T\mathbb{R}^3 \times (-\infty,\infty))$,

$$\begin{aligned}
&\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{-\infty}^{\infty} (\partial_t + v\cdot\nabla_x)\phi(x,v,t) f^{(1)}(x,v,t)\,\mathrm{d}t\,\mathrm{d}v\,\mathrm{d}x \\
&+ \int_{\mathbb{R}^3}\int_{\mathbb{R}^3\setminus B_\varepsilon(x)}\int_{\mathbb{R}^3}\int_{\mathcal{V}(x,\bar{x},v)}\int_{-\infty}^{\infty} \nabla_V \cdot (G(X,V,t)\phi(x,v,t)) \\
&\qquad \times f^{(2)}(X,V,t)\,\mathrm{d}t\,\mathrm{d}\bar{v}\,\mathrm{d}v\,\mathrm{d}\bar{x}\,\mathrm{d}x \\
&= \qquad (1.36)\\
&-\frac{1}{\sqrt{2}}\int_{\mathbb{R}^3}\int_{\mathbb{S}^2}\int_{\mathcal{V}(X)}\int_{-\infty}^{\infty}\phi(x,v,t)f^{(2)}([x,\bar{x}+\varepsilon n],[v,\bar{v}],t)(v-\bar{v})\cdot n\,\mathrm{d}t\,\mathrm{d}V\,\mathrm{d}n\,\mathrm{d}x \\
&-\int_{\mathcal{P}_\varepsilon}\int_{\partial\mathcal{V}(X)}\int_{-\infty}^{\infty}\phi(x,v,t)f^{(2)}(X,V,t)G(X,V,t)\cdot\hat{\nu}_V\,\mathrm{d}t\,\mathrm{d}\mathcal{H}(V,X)\,\mathrm{d}X, \qquad (1.37)
\end{aligned}$$

and $f^{(2)}$ satisfies equation (1.30).

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After a straightforward partition of phase space, the derivation of the BBGKY hierarchy then follows as a corollary of theorem 1.4. For more applicable results, one must have a good understanding of the admissible data. For example, in linear elastic hard sphere dynamics, this would result in the Boltzmann collision operator on the right-hand side of equation (1.36) [**20**]. The following is a quick corollary of our main result.

COROLLARY 1.6. *For any $f_0 \in C^0(\mathcal{D}) \cap L^1(\mathcal{D})$, there exists a global-in-time weak solution to the BBGKY hierarchy as given by definition 1.5.*

Before formulating the Liouville equation we state and prove some microscopic properties that are used in the derivation.

2. Properties of the microscopic dynamics

The proof of theorem 1.4 relies on transport identities for $\tau_i(X, V)$ and $\sigma_i(X, V)$. These identities are given in the case for linear elastic particles in [**20**]. Here we generalize to our case and interpret the results physically.

We first consider the results for the free dynamics.

PROPOSITION 2.1 (Transport Identity I). *Given $X \in \mathbb{R}^6$ and $V \in \mathcal{V}(X)$, let $\tau(X, V)$ be a particular event time in the dynamics determined by $\Psi_t^x(X, V)$ and $\Psi_t^v(X, V)$. Then for all $t \in (\tau_{i-1}, \tau_{i+1})$*

$$[\Phi_t^v \cdot \nabla_Y + G(\Phi_t^x, \Phi_t^v) \cdot \nabla_W]\tau(Y, W)|_{Y=\Phi_t^v, W=\Phi_t^v} = -1. \tag{2.1}$$

Proof. For ease of notation, we omit the arguments of Φ_t^x and Φ_t^v. Firstly, we note that the event time $\tau(X, V)$ can be written as [**20**]

$$\tau(X, V) = \arg\min\{s : \Phi_s^x(X, V) \in \partial\mathcal{P}_\varepsilon\}.$$

We first consider τ as a function of the data at time t, i.e. $\tilde{\tau}(\Psi_t(X, V), \Psi_t(X, V)) = \tau(X, V)$. To construct the time derivative of $\tilde{\tau}$, we appeal to the definition of the classical derivative. Indeed, let $h > 0$ and assume that $h \ll \delta$. Then, we have

$$\begin{aligned}\tau(\Psi_{t+h}^x, \Psi_{t+h}^v) &= \arg\min\{s \in (\tau_{i-1}, \tau_{i+1}) : \|\tilde{\Phi}_s^x(\Psi_{t+h}^x, \Psi_{t+h}^v)\| = \varepsilon\}\\ &= \arg\min\{s \in (\tau_{i-1}, \tau_{i+1}) : \|\tilde{\Phi}_{s-h}^x(\Psi_t^x, \Psi_t^v)\| = \varepsilon\}\\ &= \arg\min\{s + h \in (\tau_{i-1}, \tau_{i+1}) : \|\tilde{\Phi}_s^x(\Psi_t^x, \Psi_t^v)\| = \varepsilon\}.\end{aligned}$$

We have assumed that there exists a unique value $\bar{s}$ for which this is true. It follows that

$$\frac{1}{h}(\tau(\Psi_t^x, \Psi_t^v) - \tau(\Psi_{t+h}^x, \Psi_{t+h}^v)) = \frac{1}{h}(\bar{s} - (\bar{s} + h)) = -1.$$

Using results from generator theory [**14**], we find that, for $t \in (\tau_{i-1}, \tau_{i+1})$:

$$\partial_t\tau(\Psi_t^x, \Psi_t^v) = [\partial_t\Phi_t^x \cdot \nabla_Y + \partial_t\Phi_t^v \cdot \nabla_W]\,\tau(Y, W)|_{Y=\Phi_t^x, w=\Phi_t^v}.$$

By appealing to the Newton equations for the free particle dynamics, we arrive at the required result. □

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The time derivative of τ offers an insight to the geometric meaning of the result: advancing forward in time towards an event in the future decreases the time until the event proportionally. We note that for linear dynamics equation (2.1) reduces to

$$V \cdot \nabla_X \tau(X, V) = -1, \tag{2.2}$$

which is the first transport identity given in [**20**]. The second transport identity of interest involves the event maps $\sigma_\pm$ in an analogous result to the second transport identity in [**20**].

PROPOSITION 2.2 (Transport Identity II). *Given $X \in \mathbb{R}^6$ and $V \in \mathcal{V}(X)$, let σ_i be a particular event map in the dynamics determined by $\Psi_t^x(X, V)$ and $\Psi_t^v(X, V)$. Then for all $t \in (\tau_{i-1}, \tau_{i+1})$,*

$$[\Phi_t^v \cdot \nabla_Y + G(\Phi_t^x, \Phi_t^v) \cdot \nabla_W]\sigma(Y, W)|_{Y=\Psi_t^v, W=\Psi_t^v} = 0. \tag{2.3}$$

Proof. Generator theory provides a link between the time derivative of $\sigma_i(\Phi_t^x, \Phi_t^v)$ and the left-hand side of equation (2.3). We note that, by shifting in time,

$$\begin{aligned}\partial_t \sigma(\Phi_t^x, \Phi_t^v) &= \partial_t \big(\eta[\Phi_{\tau_i - t}^x(\Psi_t^x, \Psi_t^v), \Phi_{\tau_i - t}^v(\Psi_t^x, \Psi_t^v)] \\ &\quad \times \big(N[\Phi_{\tau_i - t}^x(\Psi_t^x, \Psi_t^v)] \otimes N[\Phi_{\tau_i - t}^x(\Psi_t^x, \Psi_t^v)]\big)\big) \\ &= \partial_t \left(\eta\left[\Phi_{\tau_i}^x, \Phi_{\tau_i}^v\right] N[\Phi_{\tau_i}^x] \otimes N[\Phi_{\tau_i}^x]\right) = 0,\end{aligned}$$

which completes the proof. □

The right-hand side confirms that the scattering maps are not dependent on time: they depend only on the instantaneous positions and velocities at the time of the interaction.

We can now use these microscopic properties to derive the Liouville equation in the next section.

3. Derivation of the Liouville equation

We consider the following three integrals

$$I(\Phi) = \int_{\mathcal{P}_\varepsilon} \int_{\mathcal{V}(X)} \int_{-\infty}^{\infty} f^{(2)}(X, V, t) \partial_t \Phi(X, V, t) \, \mathrm{d}t \, \mathrm{d}V \, \mathrm{d}X, \tag{3.1}$$

$$J(\Phi) = \int_{\mathcal{P}_\varepsilon} \int_{\mathcal{V}(X)} \int_{-\infty}^{\infty} f^{(2)}(X, V, t) V \cdot \nabla_X \Phi(X, V, t) \, \mathrm{d}t \, \mathrm{d}V \, \mathrm{d}X, \tag{3.2}$$

$$K(\Phi) = \int_{\mathcal{P}_\varepsilon} \int_{\mathcal{V}(X)} \int_{-\infty}^{\infty} f^{(2)}(X, V, t) \nabla_V \cdot [G(X, V, t) \Phi(X, V, t)] \, \mathrm{d}t \, \mathrm{d}V \, \mathrm{d}X, \tag{3.3}$$

which we call the time, space and velocity derivative terms respectively. The method to derive the Liouville equation in both of our examples is similar to the method

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used in [20]: we wish to find weak solutions $f^{(2)}$ to the equation

$$\mathcal{M}[f^{(2)}] = \mathcal{B}[f^{(2)}],$$

where the operator $\mathcal{M}$ is the Liouville operator associated to our choice of dynamics for point-like particles. To derive the operator on the right-hand side, we consider the Liouville operator acting on test functions $\Phi \in C_c^\infty(\mathcal{D} \times (-\infty, \infty))$. We then multiply $\mathcal{M}[\Phi(X, V, t)]$ by $f^{(2)}$ and integrate to find

$$\int_{\mathcal{P}_\varepsilon} \int_{\mathbb{R}^6} \int_{-\infty}^{\infty} f^{(2)}(X, V, t)\mathcal{M}[\Phi(X, V, t)]\,\mathrm{d}X\,\mathrm{d}V\,\mathrm{d}t = 0. \tag{3.4}$$

We then separate the phase space into parts where $f^{(2)}$ is smooth, and evaluate each of the corresponding integrals so constructed. Surface terms that arise then contribute to the collisional term on the right-hand side of the Liouville equation in its weak form.

3.1. The time derivative term

Using the flow maps Ψ_t^x and Ψ_t^v, we can write the integral $I(\Phi)$ as follows:

$$I(\Phi) = \int_{\mathcal{P}_\varepsilon} \int_{\mathcal{V}(X)} \sum_{i=-M(X,V)+1}^{N(X,V)} \int_{-\tau_i}^{-\tau_{i-1}} f_0^{(2)}(\Psi_{-t}^x, \Psi_{-t}^v)\partial_t\Phi(X, V, t)\,\mathrm{d}t\,\mathrm{d}V\,\mathrm{d}x. \tag{3.5}$$

On each interval (τ_{i-1}, τ_i) the flow is described by the free dynamics, so we may apply integration by parts, keeping in mind that evaluating $\Psi_t(X, V)$ at event times from the left or right provides a different result, and that using a compactly-supported test function Φ yields zero at $\tau_{-M} = -\infty, \tau_N = \infty$:

$$\begin{aligned} I(\Phi) = \int_{\mathcal{P}_\varepsilon} \int_{\mathcal{V}(X)} & \sum_{i=-M+1}^{N-1} \left\{ \Phi(X, V, \tau_i)(f_0^{(2)}(\Psi_{\tau_i^-}) - f_0^{(2)}(\Psi_{\tau_i^+})) \right\} \\ & - \sum_{i=-M+1}^{N} \left\{ \int_{-\tau_i}^{-\tau_{i-1}} \Phi(X, V, t)\partial_t f_0^{(2)}(\Psi_{-t}^x, \Psi_{-t}^v)\,\mathrm{d}t \right\} \mathrm{d}V\,\mathrm{d}X, \end{aligned}$$

where

$$\Psi_{\tau^-} = \lim_{t\to\tau^-} \Psi_t, \quad \Psi_{\tau^+} = \lim_{t\to\tau^+} \Psi_t,$$

meaning that the summation of the surface terms in this integral do not cancel (due to the application of σ_i at each event time τ_i). For each interval (τ_{i-1}, τ_i), the flow maps Ψ_t^x and Ψ_t^v are determined by the free dynamics Φ_t^x and Ψ_t^v. We apply the chain rule on each of these intervals. For the second term in this result, we consider three separate cases. If there are no particle–particle interactions for initial data

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X, V such that $M + N = 1$, we have that

$$\begin{aligned}\partial_t f_0^{(2)}(\Psi^x_{-t}, \Psi^v_{-t}) &= [\partial_t \Phi^x_{-t} \cdot \nabla_Y + \partial_t \Phi^v_{-t} \cdot \nabla_W] f_0^{(2)}|_{Y=\Phi^x_{-t}, W=\Phi^v_{-t}}, \\ &= [\Phi^v_{-t} \cdot \nabla_Y + G(X, V, -t) \cdot \nabla_W] f_0^{(2)}|_{Y=\Phi^x_{-t}, W=\Phi^v_{-t}}, \\ &= -[\Psi^v_{-t} \cdot \nabla_X + G(X, V, -t) \cdot \nabla_V] f^{(2)}(X, V, t).\end{aligned}$$

For initial data which causes particle–particle collisions, we define $i_0 = 0$ if $\tau_0 < 0$ (i.e. the closest event to $t = 0$ is in the past) and $i_0 = 1$ if $\tau_0 > 0$ (the closest event is in the future). Then for $\tau_{i_0-1} \leqslant t \leqslant \tau_{i_0}$,

$$\partial_t f_0^{(2)}(\Psi^x_{-t}, \Psi^v_{-t}) = -[\Psi^v_{-t} \cdot \nabla_X + G(X, V, -t) \cdot \nabla_V] f^{(2)}(X, V, t),$$

for $\tau_i < t < \tau_{i+1}, i = i_0, \ldots, N-1$,

$$\begin{aligned}\partial_t f_0^{(2)}(\Psi^x_{-t}, \Psi^v_{-t}) = -[&\Psi^v_{-(t-\tau_i)} \cdot \nabla_Y \\ &+ G(\Psi^x_{-\tau_i}, \sigma_i^+ \Psi^v_{-\tau_i}, -(t-\tau_i)) \cdot \nabla_W] f^{(2)}(Y, W, t),\end{aligned}$$

and for $\tau_i < t < \tau_{i+1}, i = -M+1, \ldots, (i_0 - 1)$,

$$\begin{aligned}\partial_t f_0^{(2)}(\Psi^x_{-t}, \Psi^v_{-t}) = -[&\Psi^v_{-(t-\tau_i)} \cdot \nabla_Y \\ &+ G(\Psi^x_{-\tau_i}, \sigma_i^- \Psi^v_{-\tau_i}, -(t-\tau_i)) \cdot \nabla_W] f^{(2)}(Y, W, t).\end{aligned}$$

We partition the result into the surface terms and the new integrals:

$$I_1(\Phi) = \int_{\mathcal{P}_\varepsilon} \int_{\mathcal{V}(X)} \sum_{i=-M+1}^{N-1} \Phi(X, V, \tau_i)(f_0^{(2)}(\Psi_{\tau_i^-}) - f_0^{(2)}(\Psi_{\tau_i^+}))\, \mathrm{d}V\, \mathrm{d}X, \tag{3.6}$$

$$I_2(\Phi) = -\int_{\mathcal{P}_\varepsilon} \int_{\mathcal{V}(X)} \sum_{i=-M+1}^{N} \int_{-\tau_i}^{-\tau_{i-1}} \Phi(X, V, t) \partial_t f_0^{(2)}(\Psi^x_{-t}, \Psi^v_{-t})\, \mathrm{d}t\, \mathrm{d}V\, \mathrm{d}X. \tag{3.7}$$

3.2. The space derivative term

We write $J(\Phi)$ as a sum of time integrals, where for each integral the argument is smooth:

$$J(\Phi) = \int_{\mathcal{P}_\varepsilon} \int_{\mathcal{V}(X)} \sum_{i=-M+1}^{N} \int_{-\tau_i}^{-\tau_{i-1}} f_0^{(2)}(\Psi^x_{-t}, \Psi^v_{-t}) V \cdot \nabla_X \Phi(Z, t)\, \mathrm{d}t\, \mathrm{d}V\, \mathrm{d}X, \tag{3.8}$$

so that on each interval we can apply the following rule:

$$f_0^{(2)} V \cdot \nabla_X \Phi = \nabla_X \cdot (V f_0^{(2)} \Phi) - \Phi V \cdot \nabla_X f_0^{(2)}. \tag{3.9}$$

Then we have

$$\begin{aligned}J(\Phi) = \int_{\mathcal{P}_\varepsilon} \int_{\mathcal{V}(X)} \Bigg\{ &\sum_{i=-M+1}^{N} \int_{-\tau_i}^{-\tau_{i-1}} \nabla_X \cdot (V f_0^{(2)} \Phi)\, \mathrm{d}t \\ &- \int_{-\infty}^{\infty} \Phi(X, V, t) V \cdot \nabla_X f^{(2)}(X, V, t)\, \mathrm{d}t \Bigg\}\, \mathrm{d}V\, \mathrm{d}X.\end{aligned} \tag{3.10}$$

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We then consider the first (divergence) term in $J(\Phi)$. We split this integral according to regions whose velocities $V \in \mathcal{C}(X)$ cause interactions and $V \in \mathcal{V}(X)\backslash\mathcal{C}(X)$ that do not. For the latter case we have

$$M_1(\Phi) := \int_{\mathcal{P}_\varepsilon} \int_{\mathcal{V}(X)\backslash\mathcal{C}(X)} \int_{-\infty}^{\infty} \nabla_X \cdot (V f_0^{(2)}(\Phi_{-t}^x, \Phi_{-t}^v)\Phi(X,V,t))\,\mathrm{d}t\,\mathrm{d}V\,\mathrm{d}X \quad (3.11)$$

which then, by the divergence theorem yields

$$M_1(\Phi) = \int_{\partial\mathcal{P}_\varepsilon} \int_{\mathcal{V}(X)\backslash\mathcal{C}(X)} \int_{-\infty}^{\infty} \Phi(X,V,t) f^{(2)}(X,V,t) V \cdot \hat{\nu}(X,V)\,\mathrm{d}t\,\mathrm{d}V\,\mathrm{d}\mathcal{H}(X), \quad (3.12)$$

where $\hat{\nu}(X,V)$ is the outward unit normal to the surface $\partial\mathcal{P}_\varepsilon \subseteq \mathbb{R}^6$.

For the collisional integrals, we use Reynold's transport theorem [13] on each term in the sum to find

$$\begin{aligned}
&\int_{\mathcal{P}_\varepsilon} \int_{\mathcal{C}(X)} \sum_{i=-M+1}^{N} \int_{-\tau_i}^{-\tau_{i-1}} \nabla_X \cdot (V f_0^{(2)} \Phi)\,\mathrm{d}t\,\mathrm{d}V\,\mathrm{d}X \\
&\quad = \int_{\mathcal{P}_\varepsilon} \int_{\mathcal{C}(X)} \sum_{i=-M+1}^{N} \nabla_X \cdot \int_{-\tau_i}^{-\tau_{i-1}} V\Phi(X,V,t) f_0^{(2)}(\Psi_{-t})\,\mathrm{d}t\,\mathrm{d}V\,\mathrm{d}X \\
&\qquad + \int_{\mathcal{P}_\varepsilon} \int_{\mathcal{C}(X)} \sum_{i=-M}^{N} (V \cdot \nabla_X \tau_i)\Phi(X,V,\tau_i)[f_0^{(2)}(\Psi_{\tau_i^-}) - f_0^{(2)}(\Psi_{\tau_i^+})]\,\mathrm{d}V\,\mathrm{d}X.
\end{aligned} \quad (3.13)$$

Once again, we split the result $J(\Phi)$ into several parts:

$$J_1(\Phi) = \int_{\mathcal{P}_\varepsilon} \int_{\mathcal{C}(X)} \sum_{i=-M}^{N} (V \cdot \nabla_X \tau_i)\Phi(X,V,\tau_i)[f_0^{(2)}(\Psi_{\tau_i^-}) - f_0^{(2)}(\Psi_{\tau_i^+})]\,\mathrm{d}V\,\mathrm{d}X, \quad (3.14)$$

$$J_2(\Phi) = -\int_{\mathcal{P}_\varepsilon} \int_{\mathcal{V}(X)} \int_{-\infty}^{\infty} \Phi(X,V,t) V \cdot \nabla_X f^{(2)}(X,V,t)\,\mathrm{d}t\,\mathrm{d}V\,\mathrm{d}X, \quad (3.15)$$

$$\begin{aligned}
J_3(\Phi) &= \int_{\partial\mathcal{P}_\varepsilon} \int_{\mathcal{V}(X)\backslash\mathcal{C}(X)} \int_{-\infty}^{\infty} \Phi(X,V,t) f^{(2)}(X,V,t) V \cdot \hat{\nu}(X,V)\,\mathrm{d}t\,\mathrm{d}V\,\mathrm{d}\mathcal{H}(X) \\
&\quad + \int_{\partial\mathcal{P}_\varepsilon} \int_{\mathcal{C}(X)} \sum_{i=-M+1}^{N} \nabla_X \cdot \int_{-\tau_i}^{-\tau_{i-1}} V\Phi(X,V,t) f_0^{(2)}(\Psi_{-t})\,\mathrm{d}t\,\mathrm{d}V\,\mathrm{d}X.
\end{aligned} \quad (3.16)$$

3.3. The velocity derivative term

The velocity derivative follows a similar argument to the one above in that we use the following calculus identity between each two event times, as in the spatial

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derivative case:

$$f^{(2)}\nabla_V\cdot(G\Phi)=\nabla_V\cdot(Gf^{(2)}\Phi)-\Phi G\cdot\nabla_V f^{(2)}. \tag{3.17}$$

For the first term on the right-hand side of equation (3.17) we initially consider the case of no interactions. As we have assumed that for each $X\in\mathcal{P}_\varepsilon$, $\mathcal{V}(X)\backslash\mathcal{C}(X)$ is a piecewise analytic submanifold of $\mathbb{R}^6$, the divergence theorem provides us with the following result:

$$\begin{aligned} M_2(\Phi):&=\int_{\mathcal{P}_\varepsilon}\int_{\mathcal{V}(X)\backslash\mathcal{C}(X)}\int_{-\infty}^{\infty}\nabla_V\cdot(G(X,V,t)\Phi(X,V,t)f_0^{(2)}(\Phi_{-t}))\,\mathrm{d}t\,\mathrm{d}V\,\mathrm{d}X,\\ &=\int_{\mathcal{P}_\varepsilon}\int_{\partial(\mathcal{V}(X)\backslash\mathcal{C}(X))}\int_{-\infty}^{\infty}f^{(2)}(X,V,t)\Phi(X,V,t)G\cdot\hat{\eta}_V(V)\,\mathrm{d}t\,\mathrm{d}\mathcal{H}(V)\,\mathrm{d}X. \end{aligned} \tag{3.18}$$

For the collisional part, we have, using the Reynolds transport theorem in an analogous fashion to before, under the assumption that $\mathcal{C}(X)$ is an analytic submanifold of $\mathcal{V}(X)$, that:

$$\begin{aligned} &\int_{\mathcal{P}_\varepsilon}\int_{\mathcal{C}(X)}\sum_{i=-M+1}^{N}\int_{-\tau_i}^{\tau_{i-1}}\nabla_V\cdot(G\Phi f_0^{(2)}(\Psi_{-t}))\,\mathrm{d}t\,\mathrm{d}V\,\mathrm{d}X\\ &\qquad=\int_{\mathcal{P}_\varepsilon}\int_{\mathcal{C}(X)}\sum_{i=-M+1}^{N}\nabla_V\cdot\int_{-\tau_i}^{-\tau_{i-1}}Gf^{(2)}(Z,t)\Phi(Z,t)\,\mathrm{d}t\,\mathrm{d}V\,\mathrm{d}X\\ &\qquad\quad+\int_{\mathcal{P}_\varepsilon}\int_{\mathcal{C}(X)}\sum_{i=-M+1}^{N-1}[G\cdot\nabla_V\tau_i]\Phi(Z,\tau_i)[f_0^{(2)}(\Psi_{\tau_i^-})-f_0^{(2)}(\Psi_{\tau_i^+})]\,\mathrm{d}V\,\mathrm{d}X. \end{aligned} \tag{3.19}$$

We partition the result as follows:

$$K_1(\Phi)=\int_{\mathcal{P}_\varepsilon}\int_{\mathcal{C}(X)}\sum_{i=-M+1}^{N-1}[G\cdot\nabla_V\tau_i]\Phi(Z,\tau_i)[f_0^{(2)}(\Psi_{\tau_i^-})-f_0^{(2)}(\Psi_{\tau_i^+})]\,\mathrm{d}V\,\mathrm{d}X \tag{3.20}$$

$$K_2(\Phi)=-\int_{\mathcal{P}_\varepsilon}\int_{\mathcal{V}(X)}\int_{-\infty}^{\infty}\Phi(X,V,t)G\cdot\nabla_V f^{(2)}(X,V,t)\,\mathrm{d}t\,\mathrm{d}V\,\mathrm{d}X, \tag{3.21}$$

$$\begin{aligned} K_3(\Phi)&=\int_{\mathcal{P}_\varepsilon}\int_{\partial(\mathcal{V}(X)\backslash\mathcal{C}(X))}\int_{-\infty}^{\infty}f^{(2)}(X,V,t)\Phi(X,V,t)G\cdot\hat{\eta}_V(V)\,\mathrm{d}t\,\mathrm{d}\mathcal{H}(V)\,\mathrm{d}X\\ &\quad+\int_{\mathcal{P}_\varepsilon}\int_{\partial C(X)}\sum_{i=-M+1}^{N}\nabla_V\cdot\int_{-\tau_i}^{-\tau_{i+1}}Gf^{(2)}(Z,t)\Phi(Z,t)\,\mathrm{d}t\,\mathrm{d}V\,\mathrm{d}X. \end{aligned} \tag{3.22}$$

3.4. Combining all terms

We now combine all contributions into one equation. We note that, by theorem 2.1,

$$I_1(\Phi) = -(J_1(\Phi) + K_1(\Phi)), \tag{3.23}$$

and so when combining all contributions, these terms disappear.

By an application of generator theory on Ψ^x_{-t} and Ψ^v_{-t} [**14**], and the results of theorems 2.1, 2.2, we see that

$$I_2(\Phi) = -(J_2(\Phi) + K_2(\Phi)). \tag{3.24}$$

The remaining terms $J_3(\Phi)$ and $K_3(\Phi)$ are surface terms in position and velocity phase space, respectively. By applying the dominated convergence theorem [**17**], and the divergence theorem on the second term of $J_3(\Phi)$ and $K_3(\Phi)$, we find

$$J_3(\Phi) = \int_{\partial\mathcal{P}_\varepsilon}\int_{\mathcal{V}(X)}\int_{-\infty}^{\infty} f^{(2)}(X,V,t)\Phi(X,V,t)V\cdot\hat{\nu}\,\mathrm{d}t\,\mathrm{d}V\,\mathrm{d}\mathcal{H}(X), \tag{3.25}$$

$$K_3(\Phi) = \int_{\mathcal{P}_\varepsilon}\int_{\partial\mathcal{V}(X)}\int_{-\infty}^{\infty} f^{(2)}(X,V,t)\Phi(X,V,t)G(X,V,t)\cdot\hat{\nu}_V\,\mathrm{d}t\,\mathrm{d}\mathcal{H}(X,V)\,\mathrm{d}X. \tag{3.26}$$

This concludes the proof of theorem 1.4.

As previously noted, the results of theorem 1.4 are quite general. To provide more of an insight into our methodology, we now consider an example of particle dynamics and interparticle interactions that involves energy loss through collisions, external friction and a constant external spatial potential, which, for example, is of interest for modelling systems of granular media [**8**].

4. Dynamics with friction, gravity and inelasticity

4.1. Free dynamics

For some $G = [g, g] \in \mathbb{R}^6$ where $g \in \mathbb{R}^3$ and $\gamma > 0$, we consider the following differential equations:

$$\frac{\mathrm{d}\Phi^x_t(X,V)}{\mathrm{d}t} = \Phi^v_t(X,V), \quad \frac{\mathrm{d}\Phi^v_t(X,V)}{\mathrm{d}t} = -\gamma V - G. \tag{4.1}$$

Physically, these equations are used to model viscous drag and gravitational force acting on particles. The resulting paths of motion for free particles are well known and can be easily derived:

$$\Phi^x_t(X,V) = X - \frac{t}{\gamma}G + \frac{1}{\gamma}\left(V + \frac{1}{\gamma}G\right)(1 - e^{-\gamma t}), \tag{4.2}$$

$$\Phi^v_t(X,V) = -\frac{1}{\gamma}G + \left(V + \frac{1}{\gamma}G\right)e^{-\gamma t}. \tag{4.3}$$

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4.2. Inelastic collisions

We consider these dynamics where collisions between particles are *inelastic*, so that the energy of the system is reduced when two particles collide. To determine the associated scattering map, we include the following event map constraint on the forward and reverse event maps $\sigma^{\pm}$:

$$|\nabla_V \sigma^+(X,V)V| = -\alpha, \quad |\nabla_V \sigma^-(X,V)V| = -\frac{1}{\alpha} \tag{4.4}$$

We give the following result on the form of the scattering map.

LEMMA 4.1. *Under the conditions eqs.* (1.14), (1.15), (4.4), *under the additional assumption that* η *in theorem 1.2 is constant, the event maps* $\sigma^{\pm}$ *have the form*

$$\sigma^+(X,V) = I - (1+\alpha)N(X) \otimes N(X), \quad \sigma^-(X,V) = I - \frac{1+\alpha}{\alpha} N(X) \otimes N(X). \tag{4.5}$$

Proof. From theorem 1.2, we know that $\sigma^{\pm}(X,V) = I - \eta N(X) \otimes N(X)$. Then, it follows that $\nabla_V(\sigma^{\pm}(X,V)V) = I - \eta N(X) \otimes N(X)$. It remains to solve equation (4.4). As the determinant of a matrix is the product of its eigenvalues λ_i, we have that

$$\prod_{i=1}^{6} \lambda_i^+ = -\alpha, \quad \prod_{i=1}^{6} \lambda_i^- = -\frac{1}{\alpha}.$$

For both maps $\lambda_i^{\pm} = 1$ for $i = 1, \ldots, 5$, by using the 5 independent eigenvectors which are perpendicular to $N(X)$. For $\sigma^+(X,V)$, the remaining eigenvalue, associated to a vector parallel with $N(X)$, must be $-\alpha$. Thus, $V + \eta(X,V)V = -\alpha V$. Rearranging we find $\eta V = (1+\alpha)V$, which gives the required result. The result for $\sigma^-(X,V)$ is analogous. □

We remark that upon relaxing the assumption that $\eta(X,V)$ is constant, the (first) Monge–Ampère equation becomes

$$|I - N(X) \cdot V N(X) \otimes \nabla_V(\eta^+(X,V)) - \eta^+(X,V)N(X) \otimes N(X)| = -\alpha. \tag{4.6}$$

In particular, this could result in physically valid *non-linear* scattering maps $\sigma^{\pm}$ for a particular event. Understanding this equation is an interesting topic for future work. In this section we focus on the inelastic Boltzmann scattering maps defined in theorem 4.1 and note that when $\alpha = 1$ these reduce to the elastic Boltzmann scattering map considered in [**20**].

4.3. Velocity cones and collision times

As the reduced difference dynamics $\tilde{\Phi}_t^x(X,V)$ follow straight lines (parametrized exponentially in $-\gamma t$), we see that two particles satisfying eqs. (4.2), (4.3) can experience at most one collision. The initial data can be partitioned into non-interacting, pre-collisional and post-collisional cases.

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For $X \in \mathcal{P}_\varepsilon$ and $V \in \mathbb{R}^6$, we write $\mathcal{L}(X,V) \subset \mathbb{R}^6$ to denote the line

$$\mathcal{L}(X,V) = \left\{ X - \frac{gt}{\gamma} + \frac{1}{\gamma}\left(V + \frac{g}{\gamma}\right)(1 - e^{-\gamma t}) : t \in \mathbb{R} \right\}, \tag{4.7}$$

and define the two infinite half lines

$$\mathcal{L}^-(X,V) = \left\{ X - \frac{gt}{\gamma} + \frac{1}{\gamma}\left(V + \frac{g}{\gamma}\right)(1 - e^{-\gamma t}) : t \leqslant 0 \right\}, \tag{4.8}$$

$$\mathcal{L}^+(X,V) = \left\{ X - \frac{gt}{\gamma} + \frac{1}{\gamma}\left(V + \frac{g}{\gamma}\right)(1 - e^{-\gamma t}) : t \geqslant 0 \right\}. \tag{4.9}$$

The velocity collision cone is then defined analogously:

$$\mathcal{C}(X) = \left\{ V \in \mathbb{R}^6 : \mathcal{L}(X,V) \cap \partial\mathcal{P}_\varepsilon \neq \emptyset \right\}. \tag{4.10}$$

We split this set into pre-collisional and post-collisional velocities respectively:

$$\mathcal{C}^-(X) = \left\{ V \in \mathcal{C}(X) : \mathcal{L}^+(X,V) \cap \partial\mathcal{P}_\varepsilon \neq \emptyset \right\}, \tag{4.11}$$

$$\mathcal{C}^+(X) = \left\{ V \in \mathcal{C}(X) : \mathcal{L}^-(X,V) \cap \partial\mathcal{P}_\varepsilon \neq \emptyset \right\}. \tag{4.12}$$

We note that a constant external potential G does not have an effect on the shape of the collision cones, as it does not affect the dynamics determined by the relative distance of the particles. The frictional constant γ truncates the pre-collisional velocity cone (when compared to linear dynamics). However, for these dynamics, for any given $X \in \mathcal{P}_\varepsilon$, all initial velocities $V \in \mathbb{R}^6$ are admissible, and so in particular the second surface term in the weak formulation of the Liouville equation disappears.

In this case we can analytically construct the unique event time $\tau(X,V)$.

Lemma 4.2 (Characterization of the collision time map for dynamics with gravity and friction). *For any $X \in \mathcal{P}_\varepsilon$, the following statements hold:*

(i) *If $V \in \mathcal{C}^+(X)$, then $\tilde{x} \cdot \tilde{v} > 0$ and*

$$\tau(X,V) = -\frac{1}{\gamma}\log\left(1 + \frac{\gamma}{\|\tilde{v}\|}\left\{\tilde{x}\cdot\widehat{\tilde{v}} + \left[(\tilde{x}\cdot\widehat{\tilde{v}})^2 - (\|\tilde{x}\|^2 - \varepsilon^2)\right]^{1/2}\right\}\right). \tag{4.13}$$

(ii) *If $V \in \mathcal{C}^-(X)$, then $-(1/2)(\gamma(\|x\|^2 - \varepsilon^2) + (\|\tilde{v}\|^2/\gamma)) < \tilde{x}\cdot\tilde{v} < 0$ and*

$$\tau(X,V) = -\frac{1}{\gamma}\log\left(1 + \frac{\gamma}{\|\tilde{v}\|}\left\{\tilde{x}\cdot\widehat{\tilde{v}} - \left[(\tilde{x}\cdot\widehat{\tilde{v}})^2 - (\|\tilde{x}\|^2 - \varepsilon^2)\right]^{1/2}\right\}\right). \tag{4.14}$$

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Proof. The collision occurs when

$$\|\tilde{\Phi}_t^x(X,V)\|^2 = \varepsilon^2 \implies \|\tilde{x} + \frac{1}{\gamma}(\tilde{v})(1-e^{-\gamma\tau})\| = \varepsilon^2.$$

By expanding the left-hand side and rearranging, we have that if the particles collide, then $\tau(X,V)$ must take one of the two following values

$$\tau^-(X,V) = -\frac{1}{\gamma}\log\left(1 + \frac{\gamma}{\|\tilde{v}\|}\left\{\tilde{x}\cdot\widehat{\tilde{v}} - \left[(\tilde{x}\cdot\widehat{\tilde{v}})^2 - (\|\tilde{x}\|^2 - \varepsilon^2)\right]^{1/2}\right\}\right),$$
$$\tau^+(X,V) = -\frac{1}{\gamma}\log\left(1 + \frac{\gamma}{\|\tilde{v}\|}\left\{\tilde{x}\cdot\widehat{\tilde{v}} + \left[(\tilde{x}\cdot\widehat{\tilde{v}})^2 - (\|\tilde{x}\|^2 - \varepsilon^2)\right]^{1/2}\right\}\right).$$

We note that the argument in the square root requires $\tilde{x}\cdot\hat{\tilde{v}} < -(\|\tilde{x}\|^2 - \varepsilon^2)^{1/2}$ or $\tilde{x}\cdot\hat{\tilde{v}} > (\|\tilde{x}\|^2 - \varepsilon^2)^{1/2}$, and if both $\tau^\pm(X,V)$ exist, then $\tau^-(X,V) < \tau^+(X,V)$. Assume now that $V \in \mathcal{C}^+(X)$; then $\tau^\pm(X,V) < 0$, and so $\tau^+(X,V) > \tau^-(X,V)$, whence $\tau(X,V) = \tau^+(X,V)$ is required. Furthermore,

$$\tilde{x}\cdot\tilde{v} > \frac{\|\tilde{v}\|}{\gamma} + ((\tilde{x}\cdot\tilde{v})^2 - (\|\tilde{x}\|^2 - \varepsilon^2))^{1/2} > 0,$$

and so $\tilde{x}\cdot\tilde{v} > 0$. Alternatively, if $V \in \mathcal{C}^-(X)$, $\tau(X,V) > 0$ and so we take $\tau(X,V) = \tau^-(X,V)$. Thus

$$\tilde{x}\cdot\hat{\tilde{v}} + \frac{\|\tilde{v}\|}{\gamma} > ((\tilde{x}\cdot\hat{\tilde{v}})^2 - (\|\tilde{x}\|^2 - \varepsilon^2))^{1/2}.$$

Squaring both sides and rearranging, we find

$$\tilde{x}\cdot\tilde{v} > -\frac{1}{2}\left(\gamma(\|\tilde{x}\|^2 - \varepsilon^2) + \frac{\|\tilde{v}\|}{\gamma}\right).$$

□

Remark 4.3. The inequality in the pre-collisional case relates to the presence of friction in the dynamics: if particles do not have enough energy in the direction $\tilde{x}$, then the particles will never meet.

4.4. Flow maps

Given the free particle dynamics, the scattering maps, and a full characterization of the admissible data, we are now in a position to define the hard sphere flow maps T_t. We split our considerations into collision-free and collisional dynamics. For the purposes of this section we introduce the operators $\Pi_i : \mathbb{R}^{12} \to \mathbb{R}^6$ for $i = 1$ and 2, where $(\Pi_1 \circ T_t)Z$ restricts the action of T_t on Z to its first 6 entries (i.e. spatial information), and $(\Pi_2 \circ T_t)Z$ restricts the action of T_t on Z to its last 6 entries (i.e. velocity information).

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4.4.1. *Collision-free dynamics* If $(X, V) \in \{X\} \times \mathbb{R}^6 \setminus \mathcal{C}(X)$, then

$$(\Pi_1 \circ T_t)Z = X - \frac{gt}{\gamma} + \frac{1}{\gamma}\left(V + \frac{g}{\gamma}\right)(1 - e^{-\gamma t}) \tag{4.15}$$

$$(\Pi_2 \circ T_t)Z = -\frac{g}{\gamma} + \left(V + \frac{g}{\gamma}\right)e^{-\gamma t}. \tag{4.16}$$

4.4.2. *Collisional dynamics* Firstly, if $X \in \mathcal{P}_\varepsilon$ and $V \in \mathcal{C}^-(X)$, then if $-\infty < t < \tau(X, V)$,

$$(\Pi_1 \circ T_t)Z = X - \frac{gt}{\gamma} + \frac{1}{\gamma}\left(V + \frac{g}{\gamma}\right)(1 - e^{-\gamma t}), \tag{4.17}$$

$$(\Pi_2 \circ T_t)Z = -\frac{g}{\gamma} + \left(V + \frac{g}{\gamma}\right)e^{-\gamma t}, \tag{4.18}$$

and if $\tau(X, V) < t < \infty$, then

$$(\Pi_1 \circ T_t)Z = \left[X - \frac{g\tau}{\gamma} + \frac{1}{\gamma}\left(V + \frac{g}{\gamma}\right)(1 - e^{-\gamma\tau})\right] - \frac{g(t-\tau)}{\gamma} \tag{4.19}$$

$$+ \frac{1}{\gamma}\left[\sigma_-\left((V + \frac{g}{\gamma})e^{-\gamma\tau} - \frac{g}{\gamma}\right) + \frac{g}{\gamma}\right](1 - e^{-\gamma(t-\tau)}), \tag{4.20}$$

$$(\Pi_2 \circ T_t)Z = -\frac{g}{\gamma} + \left[\sigma_-\left((V + \frac{g}{\gamma})e^{-\gamma\tau} - \frac{g}{\gamma}\right) + \frac{g}{\gamma}\right]e^{-\gamma(t-\tau)}. \tag{4.21}$$

If $X \in \mathcal{P}_\varepsilon$ and $V \in \mathcal{C}^+(X)$, then if $-\infty < t < \tau(X, V)$,

$$(\Pi_1 \circ T_t)Z = \left[X - \frac{g\tau}{\gamma} + \frac{1}{\gamma}\left(V + \frac{g}{\gamma}\right)(1 - e^{-\gamma\tau})\right] - \frac{g(t-\tau)}{\gamma} \tag{4.22}$$

$$+ \frac{1}{\gamma}\left[\sigma_+\left((V + \frac{g}{\gamma})e^{-\gamma\tau} - \frac{g}{\gamma}\right) + \frac{g}{\gamma}\right](1 - e^{-\gamma(t-\tau)}), \tag{4.23}$$

$$(\Pi_2 \circ T_t)Z = -\frac{g}{\gamma} + \left[\sigma_+\left((V + \frac{g}{\gamma})e^{-\gamma\tau} - \frac{g}{\gamma}\right) + \frac{g}{\gamma}\right]e^{-\gamma(t-\tau)}, \tag{4.24}$$

and if $\tau(X, V) < t < \infty$, then

$$(\Pi_1 \circ T_t)Z = X - \frac{gt}{\gamma} + \frac{1}{\gamma}\left(V + \frac{g}{\gamma}\right)(1 - e^{-\gamma t}), \tag{4.25}$$

$$(\Pi_2 \circ T_t)Z = -\frac{g}{\gamma} + \left(V + \frac{g}{\gamma}\right)e^{-\gamma t}. \tag{4.26}$$

Finally, if $X \in \partial\mathcal{P}_\varepsilon$,

$$(\Pi_1 \circ T_t)Z = \begin{cases} X - \frac{gt}{\gamma} + \frac{1}{\gamma}\left(V + \frac{g}{\gamma}\right)(1 - e^{-\gamma t}) & \text{if } -\infty < t < 0, \\ X - \frac{gt}{\gamma} + \frac{1}{\gamma}\left(\sigma_- V + \frac{g}{\gamma}\right)(1 - e^{-\gamma t}) & \text{if } 0 < t < \infty, \end{cases} \tag{4.27}$$

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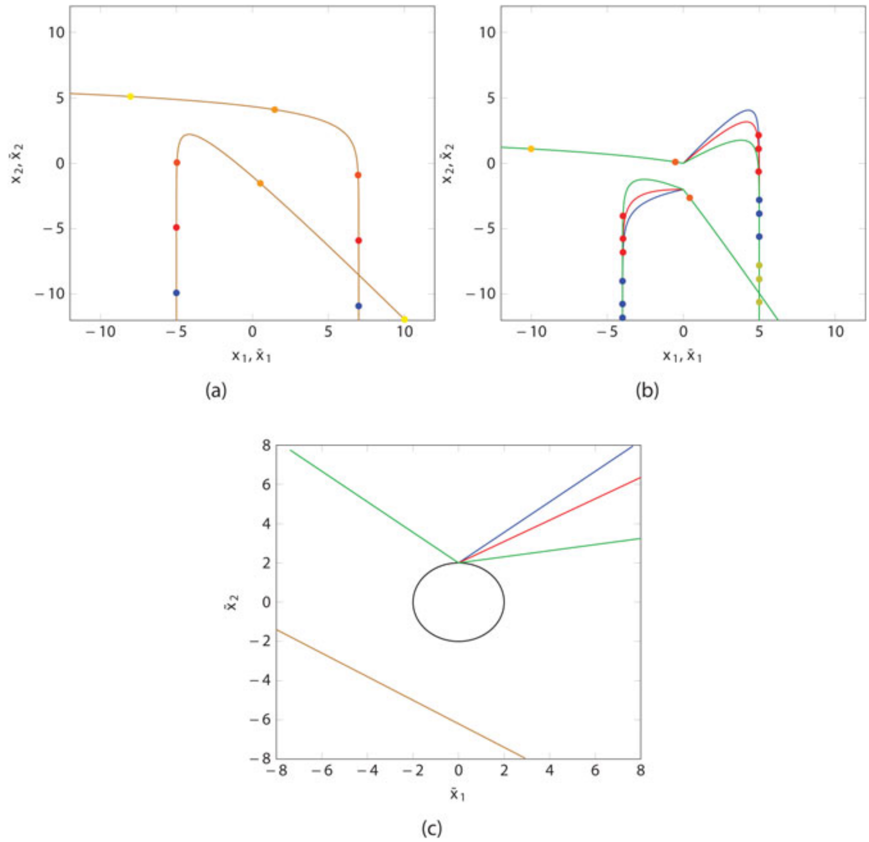

Fig. 1 - Colour online, B/W in print

Figure 1. Example trajectories of particles that are affected by gravity, friction and collide with different coefficients of restitution α. (a) Trajectories of two particles that never collide. (b) Trajectories where two particles collide with $\alpha = 1$ (blue), $\alpha = 0.7$ (red) and $\alpha = 0.2$ (green). The coloured dots on each trajectory represent the position at a particular time t. Figure 1(c) shows the same trajectories (using the same colours) considered in the reduced difference space $\tilde{x}$, where the black circle is the boundary $\partial\mathcal{P}_\varepsilon$.

and

$$(\Pi_2 \circ T_t)Z = \begin{cases} -\frac{g}{\gamma} + \left(V + \frac{g}{\gamma}\right) e^{-\gamma t} & \text{if } -\infty < t < 0, \\ -\frac{g}{\gamma} + \left(\sigma_- V + \frac{g}{\gamma}\right) e^{-\gamma t} & \text{if } 0 < t < \infty. \end{cases} \tag{4.28}$$

Two-dimensional diagrams of the trajectories that can occur in this system of dynamics is provided in figure 1, with the result in three dimensions being similar. We note that in figure 1a, although the trajectories overlap, the particles do not collide as they reach the intersection point at different times.

4.5. The Liouville equation

Using theorem 1.4, as we have characterized the admissible data X, V for the particle dynamics, we can write down the Liouville equation for these particular

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dynamics. For any $f_0^{(2)} \in C^0(\mathcal{D}) \cap L^1(\mathcal{D})$ by theorem 1.4, there exists a physical global in time weak solution of

$$\left[\frac{\partial}{\partial t} + V \cdot \nabla_X - G \cdot \nabla_V - \nabla_V \cdot (\gamma V)\right] f^{(2)}(X, V, t) = \mathcal{B}_X[f^{(2)}], \tag{4.29}$$

where the scattering map defining collisions satisfies equation (4.4).

4.6. The BBGKY hierarchy

We define $f^{(1)}(x, v, t)$ as in theorem 1.6, which then satisfies (by using $G = [g, g]$),

$$\int_{\mathcal{P}_\varepsilon} \int_{\mathbb{R}^6} \int_{-\infty}^{\infty} (\partial_t + v \cdot \nabla_x + g \cdot \nabla_v)\phi(x, v, t) f^{(1)}(x, v, t) \, \mathrm{d}t \, \mathrm{d}V \, \mathrm{d}X$$
$$= -\frac{1}{\sqrt{2}} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} \int_{\mathbb{R}^6} \int_{-\infty}^{\infty} \phi(x, v, t) f^{(2)}([x, x + \varepsilon n], [v, \bar{v}], t)(v - \bar{v}) \cdot n \, \mathrm{d}t \, \mathrm{d}V \, \mathrm{d}n \, \mathrm{d}x.$$

The collisional term $\mathcal{B}_X[f^{(2)}]$ in the above equation can then be separated into a pre-collisional and a post-collisional term:

$$\begin{aligned}\mathcal{B}_X[f^{(2)}] = {} & \frac{1}{\sqrt{2}} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} \int_{\mathcal{C}^-(X)} \int_{-\infty}^{\infty} \phi(x, v, t) f^{(2)}([x, x + \varepsilon n], [v, \bar{v}], t) \\ & \times (v - \bar{v}) \cdot n \, \mathrm{d}t \, \mathrm{d}V \, \mathrm{d}n \, \mathrm{d}x \\ & - \frac{1}{\sqrt{2}} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} \int_{\mathcal{C}^+(X)} \int_{-\infty}^{\infty} \phi(x, v, t) f^{(2)}([x, x + \varepsilon n], [v, \bar{v}], t) \\ & \times (v - \bar{v}) \cdot n \, \mathrm{d}t \, \mathrm{d}V \, \mathrm{d}n \, \mathrm{d}x,\end{aligned}$$

where

$$\mathcal{C}^+(n) = \{V \in \mathbb{R}^6 : (v - \bar{v}) \cdot n > 0\},$$

and

$$\begin{aligned}\mathcal{C}^-(n) &= \{V = [v, \bar{v}] \in \mathbb{R}^6 : -\frac{\|v - \bar{v}\|^2}{2\gamma} < (v - \bar{v}) \cdot n < 0\} \\ &= \{V = [v, \bar{v}] \in \mathbb{R}^6 : (v - \bar{v}) \cdot n < 0\},\end{aligned}$$

where the lower bound has disappeared because we are considering $X \in \partial\mathcal{P}_\varepsilon$. We introduce the change of variables for the post-collisional integral that is motivated by the backward time scattering map:

$$V \mapsto \left(I - \frac{1 + \alpha}{2\alpha} \{n \ \ -n\} \otimes \{n \ \ -n\}\right) V.$$

This transform has Jacobian $1/\alpha$. We note that

$$(v_n' - \bar{v}_n') \cdot n = -\frac{1}{\alpha}(v - \bar{v}) \cdot n,$$

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where the primed values are determined by the backward time Boltzmann inelastic scattering map, which in terms of $v, \bar{v}$ is the inverse inelastic collision rule

$$v'_n = v - \frac{1+\alpha}{2\alpha}(n \cdot (v - \bar{v}))n, \tag{4.30}$$

$$\bar{v}'_n = v + \frac{1+\alpha}{2\alpha}(n \cdot (v - \bar{v}))n, \tag{4.31}$$

and so we obtain the inelastic collision operator in the first equation of the BBGKY hierarchy:

$$\int_{\partial \mathcal{P}_\varepsilon} \int_{\mathbb{R}^6} \int_{-\infty}^{\infty} \Phi(X, V, t) f^{(2)}(X, V, t) V \cdot \tilde{\nu}(X) \, \mathrm{d}t \, \mathrm{d}V \, \mathrm{d}X, \tag{4.32}$$

$$= \frac{1}{\sqrt{2}} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} \int_{\mathcal{C}^+(n)} \int_{-\infty}^{\infty} \Phi(x, v, t) \bigg[f^{(2)}(x, v, x + \varepsilon n, \bar{v}, t) \tag{4.33}$$

$$- \frac{1}{\alpha^2} F^{(2)}(x, v', x + \varepsilon n, \bar{v}', t) \bigg] (v - \bar{v}) \cdot n \, \mathrm{d}t \, \mathrm{d}V \, \mathrm{d}n \, \mathrm{d}x.$$

We note that, under additional assumptions (i.e. molecular chaos), this is a weak analogue of the inelastic Boltzmann collision operator for particles of diameter ε.

4.7. Extension to general external and interaction potentials

In this example, as the relative trajectory of the particles is linear, two particles can only experience one event, namely the inelastic collision. By including more complicated smooth interaction potentials (e.g. a quadratic interaction potential which attracts particles to one another), multiple collisions can occur between two particles. The resulting Lioville equation will still be described by equation (1.30), under the condition that the collisions that particles experience are well separated.

Alternatively, multiple events can occur between particles by including additional interaction diameters where non-collisional events can occur. We now present an example where multiple instantaneous interactions can occur between two particles.

5. Square-shoulder particle dynamics

We now include an additional interaction diameter $\varepsilon_1 > \varepsilon > 0$, where particle trajectories are refracted away from one another, provided they can overcome an energy barrier. If the particles do not have enough energy to overcome the barrier, then they are instead reflected away. Such dynamics are sometimes considered by including a discrete interaction potential:

$$G(\|\tilde{x}\|) = \begin{cases} \infty, & \|x - \bar{x}\| < \varepsilon, \\ a, & \varepsilon < \|x - \bar{x}\| < \varepsilon_1, \\ 0, & \|x - \bar{x}\| > \varepsilon_1, \end{cases} \tag{5.1}$$

where $a > 0$. The potential is shown in figure 2.

As an alternative to using a discrete interaction potential, we will construct a new interaction type that takes place at the interaction boundary ε_1.

Fig. 2 - Colour online, B/W in print

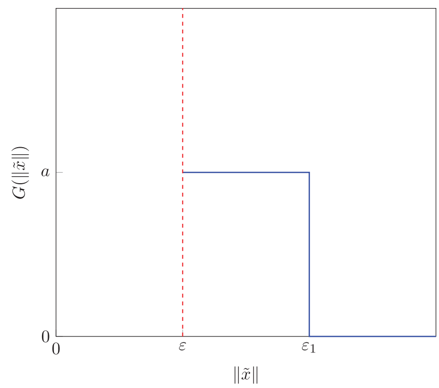

Figure 2. The step potential that is considered for this system of particles. The dashed line at $\|\tilde{x}\| = \varepsilon$ represents the hard core of the particle.

5.1. Free dynamics

For this example we will consider linear particle dynamics:

$$\frac{\mathrm{d}\Phi_t^x(X,V)}{\mathrm{d}t} = \Phi_t^v(X,V), \quad \frac{\mathrm{d}\Phi_t^v(X,V)}{\mathrm{d}t} = 0. \tag{5.2}$$

The free dynamics of the system are then given by

$$\Phi_t^x(X,V) = X + Vt, \tag{5.3}$$

$$\Phi_t^v(X,V) = V. \tag{5.4}$$

By considering linear dynamics we can fully characterize all possible trajectories of particles. However, we stress that a full characterization of all trajectories is not necessary to construct the Liouville equation, so more general external and interaction potentials may also be considered, provided there is a firm understanding of the admissible data for the system.

5.2. Particle interactions

5.2.1. *Elastic collisions* At the core interaction diameter ε, we will consider elastic collision interactions given by equation (4.5) with $\alpha = 1$. When $\alpha \neq 1$, the derivation should be similar, with some additional consideration of valid admissible intial data.

5.2.2. *Particle refractions* At the interaction diameter $\varepsilon_1 > \varepsilon > 0$, we construct a refractive boundary depending on the kinetic energy in the direction of the collision, the particles will undergo a collision or a refraction. For $X \in \partial\mathcal{P}_{\varepsilon_1} = \{[x,\bar{x}] \in \mathbb{R}^6 : \|\tilde{x}\| = \varepsilon_1\}$, there are three possible cases:

(i) $\tilde{v} \cdot \tilde{x} < 0$ and $|\tilde{v} \cdot \hat{\tilde{x}}|^2 < a$. In this case, the two particles are moving towards each other, but the energy in the direction of the interaction is not large enough to overcome the energy barrier, so the particles undergo an elastic collision.

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(ii) $\tilde{v} \cdot \tilde{x} < 0$ and $|\tilde{v} \cdot \hat{\tilde{x}}|^2 > a$. Here the particles are moving towards each other and have enough energy to overcome the barrier, so the particles continue towards each other but their velocity in the direction of the interaction is reduced.

(iii) $\tilde{v} \cdot \tilde{x} > 0$. In this case, the particles are moving away from one another. As the energy difference in this direction is negative, the particles are always refracted, and their velocities are increased in the direction of the interaction diameter.

For case 1, we can use the collision rule equation (4.5) with $\alpha = 1$. In cases 1 and 3 we require a new event rule which provides the correct dynamics: η^+ and η^- should change the speed of colliding particles in a collision, proportional to the energy barrier and the speed of the incoming particles. For these reasons we propose that

$$\eta^+ = -\frac{\|(N \otimes N)V\| - \varepsilon_1^2 a}{\|(N \otimes N)V\|}\eta^-. \tag{5.5}$$

This leads to the following definition of $\eta_\pm$:

$$\eta^+ = -\left(1 - \frac{\|(N \otimes N)V\| - \varepsilon_1^2 a}{\|(N \otimes N)V\|}\right), \quad \eta^- = -\left(1 - \frac{\|(N \otimes N)V\|}{\|(N \otimes N)V\| - \varepsilon_1^2 a}\right).$$

In terms of incoming and outgoing velocities of individual particles, this event is written as

$$\begin{aligned} v' &= v - \frac{1}{2}\left[\tilde{v} \cdot \hat{\tilde{x}} - \operatorname{sign}\left(\tilde{v} \cdot \hat{\tilde{x}}\right)\left(\left(\tilde{v} \cdot \hat{\tilde{x}}\right)^2 - a\right)^{1/2}\right]\hat{\tilde{x}}, \\ \bar{v}' &= \bar{v} + \frac{1}{2}\left[\tilde{v} \cdot \hat{\tilde{x}} - \operatorname{sign}\left(\tilde{v} \cdot \hat{\tilde{x}}\right)\left(\left(\tilde{v} \cdot \hat{\tilde{x}}\right)^2 - a\right)^{1/2}\right]\hat{\tilde{x}}. \end{aligned}$$

For $a = 0$, this equation reduces to $V' = V$, i.e. the particles do not interact. When $a > 0$, the particles lose energy of order a in the direction of the outward normal of $\partial\mathcal{P}_{\varepsilon_1}$. We can see that when $(\tilde{v} \cdot \hat{\tilde{x}})^2 < a$, the event rule cannot be applied, thus in this case we must provide an alternative event rule.

5.3. Collision times

The times at which particles reach an interaction diameter depends solely on the free dynamics. Instead of considering the collision times for individual interaction diameters, we therefore only need to consider an arbitrary diameter $\hat{\varepsilon} > 0$. Under the assumption that the particles do reach a distance $\hat{\varepsilon}$ from one another given initial conditions $X \in \mathcal{P}_\varepsilon$, $V \in \mathbb{R}^6$, we have to find the time τ where

$$\tau(X, V) = \min_{t \in \mathbb{R}}\left\{\|\tilde{\Phi}_t^x(X, V)\| = \hat{\varepsilon}\right\}. \tag{5.6}$$

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By using equation (5.3), we find that if $V \in \mathcal{C}^-(X)$ then

$$\tau(X,V) = \min_{t\in\mathbb{R}} \left\{ t = -\frac{1}{\|\tilde{v}\|}\left[-\hat{\tilde{v}}\cdot\tilde{x} \pm \left[(\hat{\tilde{v}}\cdot\tilde{x})^2 - (\|\tilde{x}\|^2 - \hat{\varepsilon}^2)\right]^{1/2}\right] : t > 0 \right\}, \quad (5.7)$$

and if $V \in \mathcal{C}^+(X)$, then

$$\tau(X,V) = \max_{t\in\mathbb{R}} \left\{ t = -\frac{1}{\|\tilde{v}\|}\left[-\hat{\tilde{v}}\cdot\tilde{x} \pm \left[(\hat{\tilde{v}}\cdot\tilde{x})^2 - (\|\tilde{x}\|^2 - \hat{\varepsilon}^2)\right]^{1/2}\right] : t < 0 \right\}. \quad (5.8)$$

Depending on the initial data, one can then determine all event times between the particles by taking $\hat{\varepsilon} = \varepsilon_1$ or $\hat{\varepsilon} = \varepsilon$, and ordering the events accordingly.

5.4. Flow maps

Given the collision times $\tau(X,V)$ for all initial data $X \in \mathcal{P}_\varepsilon$, $V \in \mathbb{R}^6$, it is then possible to construct flow maps for every possible pair of trajectories for two particles, based on eqs. (1.25)– (1.27) in a similar approach to §§ 4.4. We reduce notational burden by omitting the precise details of the flow maps, and including an overview of the types of trajectories that can occur. A diagram of the possible trajectories is then given in figure 3, along with the corresponding trajectories in the reduced difference phase space in figure 4.

We define the subset of initial data that has an interaction with the surface $\partial\mathcal{P}_{\varepsilon_1}$ as

$$\mathcal{C}_1(X) = \{V \in \mathbb{R}^6 : \exists t \in \mathbb{R} : \|\tilde{\Psi}^x_t\| = \varepsilon_1\}. \quad (5.9)$$

5.4.1. *Collision-free dynamics* For $X \in \mathcal{P}_{\varepsilon_1}$ and $V \in \mathbb{R}^6 \backslash C_1(X)$, the two particles never reach the interaction perimeter $\partial\mathcal{P}_{\varepsilon_1}$, so their dynamics are described by the free dynamics eqs. (5.3), (5.4).

5.4.2. *External bounce* When $X \in \mathcal{P}_{\varepsilon_1}$ and $V \in \mathcal{C}_1(X)$ such that $(\tilde{v}\cdot\tilde{x})^2 < a$, the particles experience a single elastic collision at the boundary $\partial\mathcal{P}_{\varepsilon_1}$ and are reflected away from one another.

5.4.3. *Refractive dynamics* For all other initial data, i.e. either $X \in \mathcal{P}_\varepsilon \backslash \mathcal{P}_{\varepsilon_1}$ and $V \in \mathbb{R}^6$, or $X \in \mathcal{P}_{\varepsilon_1}$ and $V \in \mathcal{C}_1(X)$ such that $(\tilde{v}\cdot\tilde{x})^2 > a$, there are two possible trajectory types:

(i) The particles are refracted at the boundary $\partial\mathcal{P}_{\varepsilon_1}$ at time τ_0, with outgoing velocity $\Psi^v_{\tau_0}(X,V)$ such that $\Psi^v_{\tau_0}(X,V) \in \mathbb{R}^6 \backslash \mathcal{C}(\Psi^x_{\tau_0}(X,V))$. In this case the particles will experience a further refraction event at time τ_1 when leaving the space $\mathcal{P}_\varepsilon \backslash \mathcal{P}_{\varepsilon_1}$;

(ii) The particles are refracted at the boundary $\partial\mathcal{P}_{\varepsilon_1}$ at time τ_0, with outgoing velocity $\Psi^v_{\tau_0}(X,V)$ such that $\Psi^v_{\tau_0}(X,V) \in \mathcal{C}(\Psi^x_{\tau_0}(X,V))$. The particles will then experience a core collision at time τ_1, before leaving the space $\mathcal{P}_\varepsilon \backslash \mathcal{P}_{\varepsilon_1}$ at time τ_2 and experiencing a final refraction at the perimeter $\partial\mathcal{P}_{\varepsilon_1}$.

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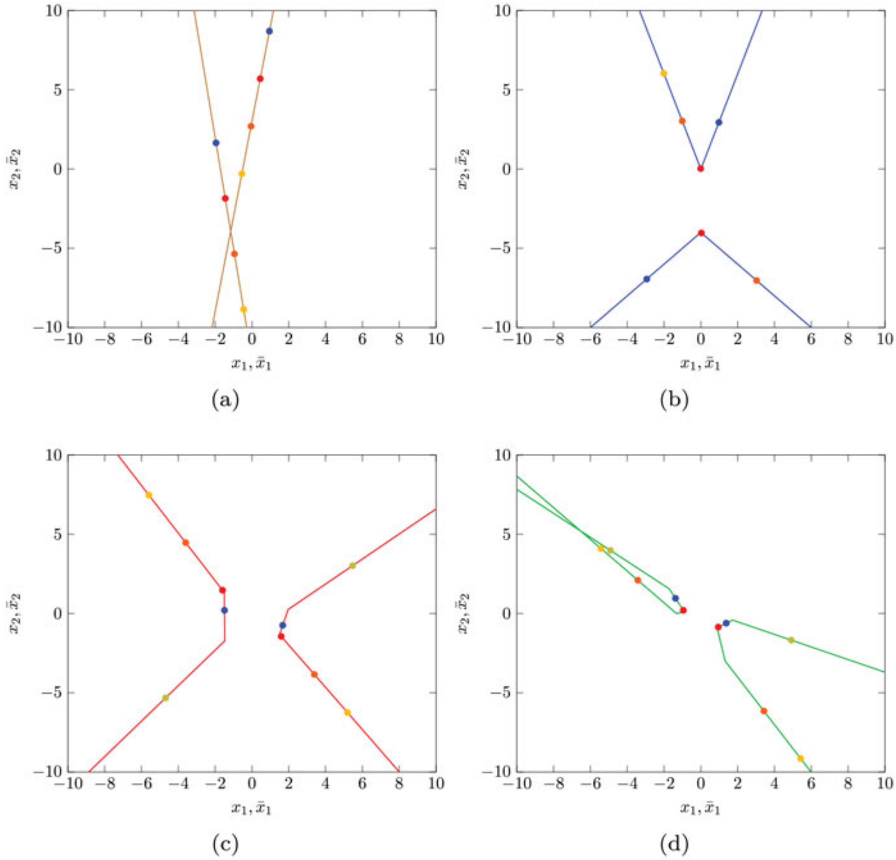

Fig. 3 - Colour online, B/W in print

Figure 3. Example trajectory pairs between two square-shoulder particles. (a) Trajectories of two particles that do not collide. (b) Trajectories where two particles experience an elastic collision at the external interaction diameter. (c) The two particles experience two refraction events. (d) The two particles experience a refraction, an elastic collision with the interior interaction diameter and a further refraction event. Each trajectory has a number of coloured points to display the location of particles at particular times t.

We consider these two interactions together as we shall see that they provide the same contribution to the Liouville equation.

5.5. The Liouville equation

To construct the Liouville equation, we partition the space of admissible initial data into three parts, then sum the corresponding contributions to derive the Liouville equation for square-shoulder particles.

5.5.1. *Collision-free dynamics* We consider trajectories where $X \in \mathcal{P}_{\varepsilon_1}$ and $V \in \mathbb{R}^6 \backslash \mathcal{C}_1(X)$. Then equation (1.30) provides us with the Liouville equation for this

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Fig. 4 - Colour online, B/W in print

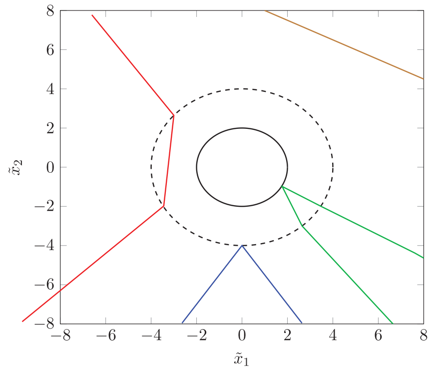

Figure 4. The corresponding reduced difference representations of the trajectories considered in figure 3. The black, solid line represents the surface $\partial\mathcal{P}_\varepsilon$ where elastic collisions take place, and the black dashed line is the surface $\partial\mathcal{P}_{\varepsilon_1}$, where particles are either refracted or reflected.

system of admissible initial data:

$$\int_{\mathcal{P}_{\varepsilon_1}}\int_{\mathbb{R}^6\backslash\mathcal{C}(X)}\int_{-\infty}^{\infty} f(X,V,t)[\partial_t\Phi(X,V,t)+V\cdot\nabla_X\Phi(X,V,t)]\,\mathrm{d}t\,\mathrm{d}V\,\mathrm{d}X = \\ -\int_{\partial\mathcal{P}_{\varepsilon_1}}\int_{\mathbb{R}^6\backslash\mathcal{C}_1(X)}\int_{-\infty}^{\infty} f(X,V,t)\Phi(X,V,t)V\cdot\hat{\nu}_X\,\mathrm{d}t\,\mathrm{d}V\,\mathrm{d}\mathcal{H}(X). \tag{5.10}$$

In this case, the collision term is zero, as for $X\in\partial\mathcal{P}_{\varepsilon_1}$, $\mathbb{R}^6\backslash\mathcal{C}_1(X)=\emptyset$.

5.5.2. *External bounce* For the set $X\in\mathcal{P}_{\varepsilon_1}$ and $V\in\{[v,\bar{x}]\in\mathbb{R}^6 : |\tilde{v}\cdot\tilde{x}|^2<a\}=:$ $\mathcal{V}_1(X)$, we have

$$\int_{\mathcal{P}_{\varepsilon_1}}\int_{\mathcal{V}_1(X)}\int_{-\infty}^{\infty} f(X,V,t)[\partial_t\Phi(X,V,t)+V\cdot\nabla_X\Phi(X,V,t)]\,\mathrm{d}t\,\mathrm{d}V\,\mathrm{d}X = \\ -\int_{\partial\mathcal{P}_{\varepsilon_1}}\int_{V_1(X)}\int_{-\infty}^{\infty} f(X,V,t)\Phi(X,V,t)V\cdot\hat{\nu}_X\,\mathrm{d}t\,\mathrm{d}V\,\mathrm{d}\mathcal{H}(X). \tag{5.11}$$

When $X\in\partial\mathcal{P}_{\varepsilon_1}$, $\mathcal{V}(X)=\{V\in\mathcal{C}_1(X) : |\tilde{v}\cdot\tilde{x}|^2<a\}$.

5.5.3. *Refractive dynamics* For dynamics where the particles have sufficient energy to overcome the barrier at ε_1 we must consider $X\in\mathcal{P}_{\varepsilon_1}$ and V in the set

$$\mathcal{V}_2(X) := \{[v,\bar{v}]\in\mathbb{R}^6 : V\in\mathcal{C}_1(X) \text{ and } |\tilde{v}\cdot\tilde{x}|^2>a \text{ if } X\in\mathcal{P}_{\varepsilon_1}\}. \tag{5.12}$$

In this case, there is more than one instantaneous interaction in the system, but by the results of theorem 1.4 we know that these interactions will not directly

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contribute to the Liouville equation. Thus, we have

$$\int_{\mathcal{P}_\varepsilon}\int_{\mathcal{V}_2(X)}\int_{-\infty}^{\infty} f(X,V,t)[\partial_t\Phi(X,V,t)+V\cdot\nabla_X\Phi(X,V,t)]\,\mathrm{d}t\,\mathrm{d}V\,\mathrm{d}X$$
$$= -\int_{\partial\mathcal{P}_\varepsilon}\int_{\mathcal{V}_2(X)}\int_{-\infty}^{\infty} f(X,V,t)\Phi(X,V,t)V\cdot\hat{\nu}_X\,\mathrm{d}t\,\mathrm{d}V\,\mathrm{d}\mathcal{H}(X). \tag{5.13}$$

For the surface integral term, when $X\in\partial\mathcal{P}_\varepsilon$, we have $V\in\mathbb{R}^6$.

5.5.4. *Combining terms* Combining the results of eqs. (5.10)–(5.11), we return the Liouville equation for square-shoulder particle dynamics:

$$\int_{\mathcal{P}_\varepsilon}\int_{\mathbb{R}^6}\int_{-\infty}^{\infty} f(X,V,t)[\partial_t\Phi(X,V,t)+V\cdot\nabla_X\Phi(X,V,t)]\,\mathrm{d}t\,\mathrm{d}V\,\mathrm{d}X$$
$$= -\int_{\partial\mathcal{P}_\varepsilon}\int_{\mathbb{R}^6}\int_{-\infty}^{\infty} f(X,V,t)\Phi(X,V,t)V\cdot\hat{\nu}_X\,\mathrm{d}t\,\mathrm{d}V\,\mathrm{d}\mathcal{H}(X)$$
$$-\int_{\partial\mathcal{P}_{\varepsilon_1}}\int_{\mathcal{V}_3(X)}\int_{-\infty}^{\infty} f(X,V,t)\Phi(X,V,t)V\cdot\hat{\nu}_X\,\mathrm{d}t\,\mathrm{d}V\,\mathrm{d}\mathcal{H}(X), \tag{5.14}$$

where

$$\mathcal{V}_3(X) := \{[v,\bar{v}]\in\mathbb{R}^6 : |\tilde{v}\cdot\tilde{x}|^2 < a\}. \tag{5.15}$$

Thus the inclusion of a square-shoulder potential term produces a partial collision operator term at the Liouville equation, and information on refraction events between particles is absorbed into the left-hand side of the equation.

We note that upon construction of the BBGKY hierarchy for square-shoulder potential systems, in addition to the standard Boltzmann collision operator given by equation (4.33), another collision term is included of the form

$$\mathcal{B}_X^a[f^{(2)}] = \frac{1}{\sqrt{2}}\int_{\mathbb{R}^3}\int_{\mathbb{S}^2}\int_{\mathcal{C}_a^+(n)}\int_{-\infty}^{\infty}\Phi(x,v,t)\Big[f^{(2)}(x,v,x+\varepsilon_1 n,\bar{v},t) \tag{5.16}$$
$$- f^{(2)}(x,v',x+\varepsilon_1 n,\bar{v}',t)\Big](v-\bar{v})\cdot n\,\mathrm{d}t\,\mathrm{d}V\,\mathrm{d}n\,\mathrm{d}x,$$

where

$$\mathcal{C}_a^+(n) = \{[v,\bar{v}]\in\mathbb{R}^6 : \tilde{v}\cdot\tilde{x} > 0 \text{ and } |\tilde{v}\cdot\tilde{x}|^2 < a\} \tag{5.17}$$

The additional contribution is due to the collisional effects at the external interaction diameter. In addition, the function $f^{(2)}$ (and in turn $f^{(1)}$) must obey a kinetic energy law on $\partial\mathcal{P}_{\varepsilon_1}$, so that it obeys equation (5.5).

6. Conclusions and future work

In this paper, we have presented derivation of the weak formulation of the Liouville equation for particles under the influence of a general dynamical form, with general

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instantaneous interactions. We have an example which is consistent with results in the literature on inelastic collision operators in the BBGKY hierarchy, and generalizes the Liouville equation for elastic hard sphere interaction. This shows the potential of the results for more complicated particle systems.

In the future, we aim to consider examples which have interactions modelled by arbitrary step potentials. This would involve considering more complicated versions of the example considered in equation (5), by using *square wells* where $a < 0$, and multiple interaction diameters ε_i. From here we can consider homogenization procedures to construct an effective potential term for particles with interactions based on step potentials, which can then be incorporated into a computational model.

The results presented could also be extended to systems with additional degrees of freedom, for example rotation or 'colour'. This would involve an analogous investigation into valid interaction types, with other conservation laws in addition to eqs. (1.14), (1.15) for the preservation of new degrees of freedom.

Finally, by investigating systems of many particles, we aim to see what initial configurations can be modelled by the Liouville equation presented here. For systems where particles experience only pairwise instantaneous interactions, we expect that for the set of admissible data which ensures that instantaneous events are well-separated, the results of this paper can be extended to systems of N particles, by partitioning the particle dynamics into subsets which can be considered as two particle systems. We also hope that the work here can motivate derivations for many-particle systems with smooth and instantaneous pairwise interactions, and that it may lead to work where the assumption that particle events are well separated can be relaxed, which for example will allow for consideration of systems that can experience inelastic collapse.

Appendix A. Tensor notation

In this paper, we also use the tensor product in several calculations. Given $A = (a_{ij})_{i=1,\ldots,n,j=1,\ldots,m} \in \mathbb{R}^{n\times m}$ and $B = (b_{ij})_{i=1,\ldots,k,j=1,\ldots,l} \in \mathbb{R}^{k\times l}$, the tensor product $A \otimes B \in \mathbb{R}^{nk\times ml}$ is given by:

$$\begin{pmatrix} a_{11}b_{11} & a_{11}b_{12} & \ldots & a_{11}b_{1l} & \ldots & \ldots & a_{1m}b_{11} & a_{1m}b_{12} & \ldots & a_{1m}b_{1l} \\ a_{11}b_{21} & a_{11}b_{22} & \ldots & a_{11}b_{2l} & \ldots & \ldots & a_{1m}b_{21} & a_{1m}b_{22} & \ldots & a_{1m}b_{2l} \\ \vdots & \vdots & \ddots & \vdots & & & \vdots & \vdots & \ddots & \vdots \\ a_{11}b_{k1} & a_{11}b_{k2} & \ldots & a_{11}b_{kl} & \ldots & \ldots & a_{1m}b_{k1} & a_{1m}b_{k2} & \ldots & a_{1m}b_{kl} \\ \vdots & \vdots & & \vdots & \ddots & & \vdots & \vdots & & \vdots \\ \vdots & \vdots & & \vdots & & \ddots & \vdots & \vdots & & \vdots \\ a_{n1}b_{11} & a_{n1}b_{12} & \ldots & a_{n1}b_{1l} & \ldots & \ldots & a_{nm}b_{11} & a_{nm}b_{12} & \ldots & a_{nm}b_{1l} \\ a_{n1}b_{21} & a_{n1}b_{22} & \ldots & a_{n1}b_{2l} & \ldots & \ldots & a_{nm}b_{21} & a_{nm}b_{22} & \ldots & a_{nm}b_{2l} \\ \vdots & \vdots & \ddots & \vdots & & & \vdots & \vdots & \ddots & \vdots \\ a_{n1}b_{k1} & a_{n1}b_{k2} & \ldots & a_{n1}b_{kl} & \ldots & \ldots & a_{nm}b_{k1} & a_{nm}b_{k2} & \ldots & a_{nm}b_{kl} \end{pmatrix}. \tag{A.1}$$

We extend the tensor products to vectors $A = (a_i)_{i=1,\ldots,n,} \in \mathbb{R}^n$ and $B = (b_i)_{i=1,\ldots,m} \in \mathbb{R}^m$ as $A \otimes B \in \mathbb{R}^{n\times m}$ where

$$A \otimes B = \begin{pmatrix} a_1b_1 & a_1b_2 & \ldots & a_1b_m \\ a_2b_1 & a_2b_2 & \ldots & a_2b_m \\ \vdots & \vdots & \ddots & \vdots \\ a_nb_1 & a_nb_2 & \ldots & a_nb_m \end{pmatrix}. \tag{A.2}$$

Tensor product notation is particularly useful when considering multidimensional derivatives of vectors in this paper; for $A \in \mathbb{R}^n$ we and a differentiable function $F : A \to \mathbb{R}^m$,we define $\nabla_A F(A) \in \mathbb{R}^{n\times m}$ as

$$\nabla_A F(A) = \begin{pmatrix} \partial_{a_1} & \partial_{a_2} & \ldots & \partial_{a_n} \end{pmatrix} \otimes F(A). \tag{A.3}$$

For example,

$$\nabla_X \tilde{x} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 & -1 \end{pmatrix} \otimes I_3, \tag{A.4}$$

where $I_3 \in \mathbb{R}^{3\times 3}$ is the identity matrix. Derivations also involve matrix vector products, and to avoid ambiguity, for a vector $a \in \mathbb{R}^n$ and matrix $b \in \mathbb{R}^{n\times n}$, we define $a \cdot B$ and $B \cdot a$ element-wise by

$$(a \cdot B)_i = \sum_{j=1}^{n} a_j B_{ji}, \quad (B \cdot a)_i = \sum_{j=1}^{n} a_j B_{ij}, \tag{A.5}$$

for $i = 1, \ldots, n$.

Appendix B. One dimensional solutions to the Monge–Ampère equation

In § 4 we introduced an event map constraint in the form of a Monge–Ampère equation equation (4.6). Under the additional assumption that $\eta(X, V)$ is a constant, we find $\eta^+(X, V) = -(1 + \alpha)$ and $\eta^-(X, V) = -\frac{(1+\alpha)}{\alpha}$. It is unclear whether other (non-linear) solutions to equation (4.6) exist. In this appendix, we produce a non-linear solution in one dimension. Firstly, in one dimension,

$$N(X) = \frac{1}{\sqrt{2}}[1, -1], \quad N(X) \otimes N(X) = \frac{1}{2}\begin{pmatrix} 1 & -1 & -1 & 1 \end{pmatrix},$$

and so

$$|D\sigma(X, V)V| = \left| \begin{pmatrix} 1 + \frac{1}{2}(v - \bar{v})\partial_v \eta + \frac{\eta}{2} & \frac{1}{2}(v - \bar{v})\partial_{\bar{v}} \eta - \frac{\eta}{2} \\ -\frac{1}{2}(v - \bar{v})\partial_v \eta - \frac{\eta}{2} & 1 + \frac{1}{2}(v - \bar{v})\partial_{\bar{v}} \eta + \frac{\eta}{2} \end{pmatrix} \right|. \tag{B.1}$$

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Thus, after some cancellations we have that

$$2\eta + (v - \bar{v})(\partial_v - \partial_{\bar{v}})\eta = -2(1+\alpha). \tag{B.2}$$

Here upon assuming that η is constant we see that the unique solution is $\eta = -(1+\alpha)$. If we write $\eta(X, V) = \eta(\tilde{v})$, then

$$\eta + \tilde{v}\partial_{\tilde{v}}\eta = -(1+\alpha). \tag{B.3}$$

Then for any $c \in \mathbb{R}$,

$$\eta = \frac{c}{\tilde{v}} - (1+\alpha) \tag{B.4}$$

is a solution of equation (4.6). As we require $\sigma^-(X, V)\sigma^+(X, V) = I$, we have that

$$\eta^+(X, V) = \frac{c}{\tilde{v}} - (1+\alpha), \quad \eta^-(X, V) = \frac{\tilde{v}}{c - \alpha\tilde{v}} - 1. \tag{B.5}$$

We note that if $\tilde{v} = c/\alpha$, $\eta^-(X, V)$ is not defined, so these scattering maps can only be applied on a restricted set of initial data. However, existence of a non-linear solution to equation (4.6) encourages further investigation.

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References

1 R. Balescu. *Equilibrium and nonequilibrium statistical mechanics* (New York: Wiley, 1975).

2 M. Bannerman and L. Lue. Exact on-event expressions for discrete potential systems. *J. Chem. Phys.* **133** (2010), 124506–12.

3 F. Cecconi, P. Tarazona and U. Marini-Bettolo-Marconi.. Theory of thermostatted inhomogeneous granular fluids: A self-consistent density functional description. *J. Chem. Phys.* **126** (2007), 1–13.

4 C. Cercigani. *The Boltzmann equation* (New York: Springer, 1988).

5 A. Donev, F. H. Stillinger and S. Torquato. Neighbor list collision-driven molecular dynamics simulation for nonspherical hard particles. *J. Comput. Phys.* **202** (2005), 765–793.

6 L. C. Evans and R. F. Gariepy. *Measure theory and fine properties of functions* (London: Chapman and Hall, 2015).

7 I. Gallagher, L. Saint-Raymond and B. Texier. From Newton to Boltzmann: hard spheres and short range potentials. Preprint, arXiv:1208.5753, 2012.

8 B. D. Goddard, T. D. Hurst and R. Ocone. Modelling inelastic granular media using Dynamical Density Functional Theory. Preprint, arXiv:2003.07327, 2020.

9 B. D. Goddard, S. Kalliadasis, A. Nold, G. A. Pavliotis and N. Savva.. General dynamical density functional theory for classical fluids. *Phys. Rev. Lett.* **109** (2012), 1–5.

10 K. Huang. *Statistical mechanics* (New York: Wiley, 1987).

11 E. M. Lifshitz and L. P. Pitaevskii. *Physical kinetics* (Oxford: Butterworth Heinemann, 1981).

https://doi.org/10.1017/prm.2020.49 Published online by Cambridge University Press

12 C. K. K. Lun, S. B. Savage, D. J. Jeffrey and N. Chepurniy.. Kinetic theories for granular flow: inelastic particles in Couette flow and slightly inelastic particles in a general flowfield. *J. Fluid Mech.* **140** (1984), 223–256.

13 J. E. Marsden, A. Tromba. *Vector calculus* (London: Macmillan, 2003).

14 G. A. Pavliotis, A. M. Stuart. *Multiscale methods: averaging and homogenization* (New York: Springer Science & Business Media, 2008).

15 F. Radjaï, F. Dubois. *Discrete-element modeling of granular materials* (New Jersey: Wiley-Iste, 2011).

16 H. Risken. *Fokker-Planck equation* (Berlin Heidelberg: Springer, 1996).

17 H. L. Royden. *Real analysis* (London: Macmillan, 1988).

18 T. Schlick. *Molecular modeling and simulation: an interdisciplinary guide* (New York: Springer Science & Business Media, 2010).

19 S. Simonella. BBGKY hierarchy for hard sphere systems. Ph.D. thesis. Sapienza University of Rome, 2011.

20 M. Wilkinson. On global-in-time chaotic weak solutions of the Liouville equation for hard spheres. Preprint, arXiv:1807.01017, 2018.