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Theory of collisional invariants for the Master kinetic equation

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ABSTRACT

The paper investigates the integral conservation properties of the Master kinetic equation, which provides an exact kinetic statistical description for the Boltzmann–Sinai classical dynamical system. It is proved that, besides the customary Boltzmann collisional invariants, this equation admits also a class of generalized collisional invariants (GCI). The result applies only when the number N and the diameter σ of hard-spheres are finite. This includes the case of dilute gases for which suitable asymptotic ordering conditions hold. However, when the Boltzmann–Grad limit is performed on the Master kinetic equation, it is shown that the existence of GCI is not permitted anymore.

1. Introduction

In this paper the problem is posed of investigating key consequences of the emerging new axiomatic "ab initio" approach to classical statistical mechanics (CSM) recently established [1–3], which led to the discovery of a non-asymptotic exact kinetic equation, to be identified with the Master kinetic equation [4]. Such an equation, whose properties are recalled below, applies to the statistical description of a classical dynamical system (CDS) realized by the Boltzmann–Sinai CDS (S_N-CDS). This is associated with a system of N identical finite-size homogeneous and rigid spherical particles, each having a constant diameter σ and immersed in a bounded subset of configuration space having rigid and stationary boundaries. The spheres are intended as hard, elastic and smooth with respect to all possible collisions which they can undergo [1]. These include arbitrary unary, binary as well as multiple collisions, in which one or more particles can interact simultaneously among themselves and/or with the boundary [1,5–7]. As shown in Ref. [1], the S_N-CDS is defined only provided the parameters N and σ are both considered as finite, namely such that $N<\infty$ and $\sigma>0$ respectively. Nevertheless, the same parameters N and σ can still satisfy suitable asymptotic orderings, which correspond to precise configurations of physical interest. These are referred to respectively as *granular fluid* and *dilute gas* (or rarefied gas) *asymptotic ordering*. The first case is prescribed by requiring

$$N \equiv \frac{1}{\varepsilon} \gg 1,\qquad \sigma \sim O(\varepsilon^0), \tag{1}$$

and the second one by letting

$$N \equiv \frac{1}{\varepsilon} \gg 1,\qquad \sigma \ll 1,\qquad K_n \sim O(\varepsilon^0). \tag{2}$$

Here $K_n \equiv N\sigma^2$ denotes the Knudsen number, implying therefore that in the dilute gas asymptotic ordering the molecular diameter σ is of $O(\varepsilon^{1/2})$.

The Master kinetic equation realizes a statistical description for hard-sphere systems described in terms of the S_N-CDS. Hence, the same kinetic equation provides a rigorous statistical treatment of the molecular dynamics occurring in these systems for arbitrary finite values of N and σ in the sense indicated above.

Regarding the continuum limit when Eqs. (2) apply in particular, as shown in Refs. [4,3] the Master kinetic equation was found to recover the customary Boltzmann kinetic equation when the Boltzmann–Grad limit is taken (see discussion below in Section 4). Nevertheless, the statistical treatment on which the new kinetic equation is based departs in fundamental ways from the traditional approach which, starting from the Boltzmann original paper [8], has been widely adopted in the literature [9–12]. The reasons are as follows. The first one concerns the functional setting of the N-body probability density function (PDF), which now

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includes both stochastic and deterministic PDFs, namely ordinary functions and distributions [1]. The second one is the physical choice adopted for the collision boundary conditions (CBC), which determine the dynamical evolution of the N-body PDF across arbitrary collision events. In contrast with the customary choice starting from Boltzmann and based on the PDF-conserving boundary conditions [11–13], the Master kinetic equation is built on the modified collision boundary conditions discussed in Ref. [2] (MCBC, see also the definition recalled below). As a consequence of such a prescription, the equation applies to arbitrary dense and rarefied systems for which the finite-size of the constituent particles must be accounted for [3]. Nevertheless, as already stated above, it recovers the Boltzmann equation in the Boltzmann–Grad limit in which particles are effectively treated as point-like [11,14–17].

In this connection, a fundamental problem which lies at the very foundation of CSM consists in the determination of the collisional invariants (CI) [8,18,19] which characterize the Master kinetic equation. Their precise knowledge in fact is a prerequisite required for the construction of the corresponding fluid statistical description. The identification of the CI depends in turn on the specific form considered for the statistical equation advancing in time the kinetic PDF. Notice that, on general grounds, the latter can in principle be assumed to be realized in terms of an evolution equation of the type

$$L_1\rho_1(\mathbf{x}_1,t)=\mathcal{C}_1. \tag{3}$$

Here $\rho_1(\mathbf{x}_1,t)$ identifies the kinetic PDF parametrized in terms of the Newtonian state $\mathbf{x}_1\equiv(\mathbf{r}_1,\mathbf{v}_1)$ spanning the 1-body phase space $\Gamma_{1(1)}=\Omega_{1(1)}\times U_{1(1)}$, with $\Omega_{1(1)}\equiv\Omega_1\subset\mathbb{R}^3$ and $U_{1(1)}\equiv\mathbb{R}^3$ being respectively the 1-body Euclidean configuration and velocity spaces. Hence, the vectors $\mathbf{r}_1$ and $\mathbf{v}_1$ can always be represented in terms of the orthogonal carthesian coordinates $\mathbf{r}_1\equiv(r_{1i},i=1,2,3)$ and corresponding velocity components $\mathbf{v}_1\equiv(v_{1i},i=1,2,3)$. Furthermore, $L_1\equiv\frac{\partial}{\partial t}+\mathbf{v}_1\cdot\frac{\partial}{\partial\mathbf{r}_1}$ and $\mathcal{C}_1$ denote respectively the 1-body free-streaming operator and an appropriate collision operator. The customary definition of CI corresponding to a generic equation of the form (3) is then provided by a real phase-function $G(\mathbf{x}_1,t)$ which satisfies the integral conservation law

$$\int\limits_{U_{1(1)}} d\mathbf{v}_1 G(\mathbf{x}_1,t)\mathcal{C}_1=0. \tag{4}$$

In the literature, the identification of the complete set of independent functions $G(\mathbf{x}_1,t)$, satisfying Eq. (4) for the S_N-CDS, is well-known [18] and is based on the Boltzmann kinetic equation. In this case, in particular, $\rho_1(\mathbf{x}_1,t)$ is identified with a suitable limit function of $\rho_1^{(N)}(\mathbf{x}_1,t)$, with $\rho_1^{(N)}(\mathbf{x}_1,t)$ being the 1-body PDF. The corresponding set of CI can then be represented by means of the phase-functions

$$\{G(\mathbf{x}_1,t)\}=\left\{G_1=A,\underline{\underline{\mathbf{G}}}_2\equiv\mathbf{B}\mathbf{v}_1,G_3=Cv_1^2\right\}. \tag{5}$$

Here $\underline{\underline{\mathbf{G}}}_2\equiv\mathbf{B}\mathbf{v}_1$ is a dyadic function with components $\underline{\underline{\mathbf{G}}}_2\equiv\left(B_iv_{1j},i,j=1,3\right)$, with B_i and v_{1j} for $i,j=1,3$ denoting the corresponding orthogonal carthesian components of $\mathbf{B}$ and of the velocity vector $\mathbf{v}_1$. Furthermore A, B_i for $i=1,2,3$ and C identify arbitrary real functions of $(\mathbf{r}_1,t)$. The phase functions $G(\mathbf{x}_1,t)$ thus defined are referred to as *Boltzmann collisional invariants* (see Refs. [18,20]). Such a result has been extended in the literature to a variety of statistical equations of the type (3) (see for example Refs. [9,11]). A development along this direction, worth to be mentioned here, refers however to the modified BBGKY hierarchy which has recently been established [3] for the S_N-CDS. Such a set of equations applies in fact for the same S_N-CDS when, based on first principles, the validity of MCBC is invoked for the physically-admissible N-body PDFs. Indeed, as shown in Ref. [3] the same set of invariants has been proved to hold when C_1 is identified with the so-called 1-body modified BBGKY collision operator which is obtained in terms of the modified BBGKY hierarchy. In this paper we intend to show in particular that the existence of similar integral conservation laws, i.e., corresponding to the set (5), can be established also in case of the Master kinetic equation.

On these premises, the answer to the issue posed above must obviously depend on the specific realization considered for the collision operator $\mathcal{C}_1$ and, hence, also of the N-body PDF itself. In particular, in the case of the Boltzmann equation, namely for point-like particles, and for a generic non-Maxwellian PDF $\rho_1(\mathbf{x}_1,t)$, the existence of the collisional invariants $G(\mathbf{x}_1,t)$ (see Eq. (5)) usually follows [18,19] by noting that for them the local identity

$$G(\mathbf{r}_1,\mathbf{v}_1^{(+)},t)+G(\mathbf{r}_1,\mathbf{v}_2^{(+)},t)-G(\mathbf{r}_1,\mathbf{v}_1^{(-)},t)-G(\mathbf{r}_1,\mathbf{v}_2^{(-)},t)=0 \tag{6}$$

applies. Concerning the notation, here and in the following the $(+)$ and $(-)$ denote quantities defined respectively after and before a collision event. The proof is obtained by invoking the conservation laws of the microscopic particle collisions. For the S_N-CDS, these are realized respectively, besides the identification $G_1\equiv A(\mathbf{r}_1,t)$, with $A(\mathbf{r}_1,t)$ denoting an arbitrary real function of $(\mathbf{r}_1,t)$, by invoking the total linear momentum and total kinetic energy conservation theorems across arbitrary collision events, i.e., in the case of binary collisions between identical particles:

$$\mathbf{v}_1^{(+)}+\mathbf{v}_2^{(+)}-\mathbf{v}_1^{(-)}-\mathbf{v}_2^{(-)}=0, \tag{7}$$

$$\frac{1}{2}\left(\mathbf{v}_1^{(+)}\right)^2+\frac{1}{2}\left(\mathbf{v}_2^{(+)}\right)^2-\frac{1}{2}\left(\mathbf{v}_1^{(-)}\right)^2-\frac{1}{2}\left(\mathbf{v}_2^{(-)}\right)^2=0. \tag{8}$$

This implies that, in the two cases (7) and (8), $G(\mathbf{x}_1,t)$ must be of the form $\underline{\underline{\mathbf{G}}}_2\equiv\mathbf{B}\mathbf{v}_1$ and $G_3=Cv_1^2$, where $\mathbf{B}$ and C, just as A, are still arbitrary, respectively vector and scalar, real functions of $(\mathbf{r}_1,t)$ only. Now, assume that $G(\mathbf{x}_1,t)$ is an analytic function of $\mathbf{v}_1$ and v_1^2, to be formally considered as independent. Then it is immediate to prove that the set $\{G(\mathbf{x}_1,t)\}$ defined by Eq. (5) is also complete. In fact, perspicuously, $G(\mathbf{x}_1,t)$ can only be – at most – a linear function alternatively of $\mathbf{v}_1$ or v_1^2 respectively.

However, as shown in Ref. [3], an analogous result can be reached in the case the S_N-CDS is associated with an ensemble of N finite-size hard-spheres. In such a case the number N remains by assumption finite, so that $\rho_1(x_1,t)\equiv\rho_1^{(N)}(x_1,t)$ can be identified with the 1-body PDF, while the collision operator $\mathcal{C}_1\equiv\mathcal{C}_1(\rho_2^{(N)})$ determines the corresponding 1-body collision operator of the modified BBGKY hierarchy. In standard notation this reads

$$\begin{aligned}\mathcal{C}_1(\rho_2^{(N)})\equiv(N-1)&\int\limits_{\Gamma_{1(2)}}^{(-)} d\mathbf{x}_2\left|\mathbf{v}_{21}\cdot\mathbf{n}_{21}\right|\\&\times\delta\left(\left|\mathbf{r}_2-\mathbf{r}_1\right|-\sigma\right)\overline{\Theta}\left(\left|\mathbf{r}_2-\frac{\sigma}{2}\mathbf{n}_2\right|-\frac{\sigma}{2}\right)\\&\times\left[\rho_2^{(N)}(\mathbf{x}_1^{(+)},\mathbf{x}_2^{(+)},t)-\rho_2^{(N)}(\mathbf{x}_1,\mathbf{x}_2,t)\right].\end{aligned} \tag{9}$$

Here $\rho_2^{(N)}(\mathbf{x}_1^{(+)},\mathbf{x}_2^{(+)},t)$ and $\rho_2^{(N)}(\mathbf{x}_1,\mathbf{x}_2,t)$ denote respectively the contributions coming from outgoing and incoming sub-domains of velocity. The precise representation of the collision operator is prescribed in terms of MCBC [1]. This requirement and its physical interpretation have been earlier discussed in detail [2]. In the Lagrangian representation, assuming left-continuity of the PDF, these are realized in terms of matching conditions for the outgoing and incoming 2-body PDFs, namely respectively

$$\rho_2^{(\pm)(N)}(\mathbf{x}_1^{(\pm)}(t_i),\mathbf{x}_2^{(\pm)}(t_i),t_i)=\lim_{t\to t_i^{(\pm)}}\rho_2^{(N)}(\mathbf{x}_1(t),\mathbf{x}_2(t),t), \tag{10}$$