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A BBGKY HIERARCHY FOR THE EXTENDED KINETIC THEORY

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The extended Boltzmann equation, which considers the possibility of creation and annihilation of particles by collision events, is derived from a generalized Liouville equation through the construction of the corresponding BBGKY hierarchy. This derivation requires a generalization of the concept of probability density and reduced distribution functions for the case in which the number of particles is not preserved. This extended Boltzmann equation is compared with previously proposed models.

1. Introduction

The Boltzmann equation describes the evolution of a dilute gas whose molecules interact through binary collisions. It plays an important role in the study of a variety of physical systems, for example in electron transport in solids, radiative processes and thermonuclear fusion [1]. Recently, this kinetic equation has been extended to consider the possibility of elementary processes in which particles can be created or annihilated. The presence of a background gas interacting with the test particles has also been considered [2, 3]. Since then, a considerable amount of work has been done in order to understand how those processes modify the relaxation behaviour of the gaseous system. Polynomial series [4] and hydrodynamical approaches [5, 6], as well as simplified gas models [7, 8], have been successfully used to find the characteristic features of this extended kinetic theory.

For a single species system, whose distribution function $f(\boldsymbol{x}, \boldsymbol{v}, t)$ depends on the position $\boldsymbol{x}$, the velocity $\boldsymbol{v}$ and the time t, the generalized Boltzmann equation reads [2]

$$\left[\partial_t + \boldsymbol{v}\cdot\nabla_x + \frac{\boldsymbol{F}}{m}\cdot\nabla_v\right] f(\boldsymbol{x},\boldsymbol{v},t) = B[f,f] + L[f] + \int \mathrm{d}\boldsymbol{v}'\,\mathrm{d}\boldsymbol{w}'\,\sigma^{c}(\boldsymbol{v}'\boldsymbol{w}'\to\boldsymbol{v})f(\boldsymbol{v}')f(\boldsymbol{w}')$$

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$$+\int \mathrm{d}\boldsymbol{v}'\,\mathrm{d}\boldsymbol{w}'\,\sigma_{\mathrm{B}}^{\mathrm{c}}(\boldsymbol{v}'\boldsymbol{w}'\rightarrow\boldsymbol{v})f(\boldsymbol{v}')g(\boldsymbol{w}')$$

$$-f(\boldsymbol{v})\int \mathrm{d}\boldsymbol{w}\,\sigma^{\mathrm{r}}(\boldsymbol{v}\boldsymbol{w})f(\boldsymbol{w}) - f(\boldsymbol{v})\int \mathrm{d}\boldsymbol{w}\,\sigma_{\mathrm{B}}^{\mathrm{r}}(\boldsymbol{v}\boldsymbol{w})g(\boldsymbol{w})\,. \qquad (1.1)$$

In eq. (1.1) $\boldsymbol{F}$ is an external conservative force and m is the mass of the test particles. The bilinear operator $B[f, f]$ describes the elastic collisions between test particles and reads

$$B[f,f] = \int \mathrm{d}\boldsymbol{w}\,\mathrm{d}\boldsymbol{v}'\,\mathrm{d}\boldsymbol{w}'\,\sigma(\boldsymbol{v}\boldsymbol{w}\rightarrow\boldsymbol{v}'\boldsymbol{w}')[f(\boldsymbol{v}')f(\boldsymbol{w}') - f(\boldsymbol{v})f(\boldsymbol{w})]\,, \qquad (1.2)$$

where $\sigma(\boldsymbol{v}\boldsymbol{w}\rightarrow\boldsymbol{v}'\boldsymbol{w}')$ is the transition frequency for the binary collision $(\boldsymbol{v}, \boldsymbol{w})\rightarrow(\boldsymbol{v}', \boldsymbol{w}')$. Spatial and temporal variables have been eliminated to clarify the notation. The elastic interaction with the background gas with a previously known distribution function denoted by $g(\boldsymbol{x}, \boldsymbol{v}, t)$ is described by the operator $L[f]$, whose form is analogous to eq. (1.2), replacing $f(\boldsymbol{w})$ and $f(\boldsymbol{w}')$ by $g(\boldsymbol{w})$ and $g(\boldsymbol{w}')$, respectively.

Creation and removal processes are described by the last four terms of eq. (1.1). They respectively represent:

(1) Creation of a particle with velocity $\boldsymbol{v}$ by interaction between two test particles with velocities $\boldsymbol{v}'$ and $\boldsymbol{w}'$, characterized by a transition frequency $\sigma^{\mathrm{c}}(\boldsymbol{v}'\boldsymbol{w}'\rightarrow\boldsymbol{v})$.

(2) Creation of a particle with velocity $\boldsymbol{v}$ by interaction between a test particle with velocity $\boldsymbol{v}'$ and a background particle with velocity $\boldsymbol{w}'$, characterized by a transition frequency $\sigma_{\mathrm{B}}^{\mathrm{c}}(\boldsymbol{v}'\boldsymbol{w}'\rightarrow\boldsymbol{v})$.

(3) Removal of a test particle with velocity $\boldsymbol{v}$ by interaction with a test particle of velocity $\boldsymbol{w}$, characterized by a transition frequency $\sigma^{\mathrm{r}}(\boldsymbol{v}\boldsymbol{w})$.

(4) Removal of a particle with velocity $\boldsymbol{v}$ by interaction with a background particle of velocity $\boldsymbol{w}$, characterized by a transition frequency $\sigma_{\mathrm{B}}^{\mathrm{r}}(\boldsymbol{v}\boldsymbol{w})$.

As done by Boltzmann in 1872, when he proposed the kinetic equation, the creation and removal terms have been introduced *ad hoc* [2]. The proposed form for these terms has been based on heuristic arguments, according to the temporal evolution that the corresponding processes are expected to determine in the distribution function. A justification for that form, based on more fundamental arguments, has not been developed up to this moment.

For the original Boltzmann equation, in which only elastic binary collisions are considered, a justification from elementary mechanical laws was introduced about 1940, and it is a usual subject in textbooks on nonequilibrium statistical mechanics [9]. This justification is based on the Liouville equation, which governs the evolution of the probability density $\rho_N(x_1 \ldots x_N, t)$ for a system of

N particles, with coordinates $x_1, \ldots, x_N$ in the phase space at time t; $x_i \equiv (\boldsymbol{x}_i, \boldsymbol{p}_i)$. If $\mathcal{H}_N$ is the Hamiltonian function of the system, the Liouville equation reads

$$\partial_t \rho_N = [\mathcal{H}_N, \rho_N] , \tag{1.3}$$

where [,] indicates the Poisson brackets. The derivation of the Boltzmann equation requires a definition for the distribution function from the density ρ_N. More generally, the reduced s-particle distribution function is defined as the probability of finding s given particles with coordinates $x_1, \ldots, x_s$ $(s < N)$ at time t:

$$f_s(x_1 \ldots x_s, t) = \frac{N!}{(N-s)!} \int \mathrm{d}x_{s+1} \ldots \mathrm{d}x_N \, \rho_N(x_1 \ldots x_N, t) . \tag{1.4}$$

The numerical factor in the definition of f_s has been taken according to the following normalization for the probability density [10]:

$$\int \mathrm{d}x_1 \ldots \mathrm{d}x_N \, \rho_N = 1 , \tag{1.5}$$

which implies $f_0(t) = 1$. Furthermore, $\rho_N(x_1 \ldots x_N, t)$ being symmetric in its arguments, this symmetry is also satisfied by the reduced distribution functions. Taking the Hamiltonian describing only pair interactions, i.e.,

$$\mathcal{H}_N(x_1 \ldots x_N) = (2m)^{-1} \sum_{i=1}^{N} [\boldsymbol{p}_i^2 + U(\boldsymbol{x}_i)] + \sum_{i<j}^{N} V_{ij}(\boldsymbol{x}_i, \boldsymbol{x}_j) , \tag{1.6}$$

the Liouville equation implies the following evolution laws for the reduced distribution functions:

$$\partial_t f_s = [\mathcal{H}_s, f_s] + \int \mathrm{d}x_{s+1} \left[\sum_{i=1}^{s} V_{i\,s+1}, f_{s+1} \right] . \tag{1.7}$$

The binary interaction between particles couples f_s with f_{s+1}. The resulting chain of equations (1.7) is known as the BBGKY hierarchy [10]. A further neglect of the pair correlations in the computation of $f_2(x_1 x_2, t)$, i.e., the Boltzmann *Stosszahl ansatz*,

$$f_2(x_1 x_2, t) = f_1(x_1, t) f_1(x_2, t) , \tag{1.8}$$

enables the formulation of a nonlinear kinetic equation for the one-particle distribution function $f_1(x_1, t)$, which is precisely the Boltzmann equation [10]:

$$D_t f_1(x) = \int dx' \, dx'' \, dy \, \sigma(xx' \to x''y)[f_1(x'')f_1(y) - f_1(x)f_1(x')] , \tag{1.9}$$

with

$$D_t = \partial_t + \boldsymbol{v} \cdot \boldsymbol{\nabla}_r + \frac{\boldsymbol{F}}{m} \cdot \boldsymbol{\nabla}_v .$$

The aim of this paper is to derive the BBGKY hierarchy when creation and annihilation processes are allowed. It implies the consideration of a system whose particle number is not fixed. The definition of the probability density and the reduced distribution functions must be accordingly modified, and the effects of such processes have to be introduced at the level of the Liouville equation. From that point, evolution equations for the reduced distributions will be obtained up to the one-particle function $f(\boldsymbol{x}, \boldsymbol{v}, t)$. The hypothesis of molecular chaos, eq. (1.8), will be applied to derive the Boltzmann equation, to be compared with the previously proposed model, eq. (1.1).

2. Extended densities and Liouville equation

The first problem which we must deal with in making fundamental of the extended kinetic theory is the violation of the particle number conservation. Since N must be considered as a variable of the system, it is not possible to describe its evolution by means of a function $\rho_N(x_1 \ldots x_N, t)$ with a fixed number of variables. Instead, we introduce a density vector

$$\boldsymbol{\rho} = [\rho_0(t), \rho_1(x_1, t), \rho_2(x_1x_2, t), \rho_3(x_1x_2x_3, t), \ldots] , \tag{2.1}$$

where $\rho_n(x_1 \ldots x_n, t)$ is the probability density of finding n particles with coordinates $x_1, \ldots, x_n$ at time t. These functions are required to be symmetric in their coordinates and to satisfy the conservation of the total probability,

$$\rho_0(t) + \sum_{n=1}^{\infty} \int dx_1 \ldots dx_n \, \rho_n(x_1 \ldots x_n, t) = 1 . \tag{2.2}$$

This normalization generalizes eq. (1.5).

Regarding the reduced s-particle distribution function, we want to preserve its definition as the probability of finding s particles with coordinates $x_1, \ldots, x_s$

at time t. According to the definition of the density vector, we write

$$f_s(x_1 \dots x_s, t) = s!\rho_s(x_1 \dots x_s, t) + \sum_{n=s+1}^{\infty} \frac{n!}{(n-s)!} \int dx_{s+1} \dots dx_n \, \rho_n(x_1 \dots x_n, t)$$
$$\equiv \sum_{r=0}^{\infty} \frac{(s+r)!}{r!} \int dx_{s+1} \dots dx_{s+r} \, \rho_{s+r}(x_1 \dots x_{s+r}) \, . \quad (2.3)$$

The last line in eq. (2.3) has been introduced to simplify the notation. The reduced distribution functions satisfy the symmetry in their variables and, because of eq. (2.2), $f_0(t) = 1$. Up to here, the identification of this generalized formulation with the original conservative problem is straightforward.

In order to introduce the extended Liouville equation, we must evaluate the effects of the creation and removal processes at a microscopic level on the evolution of the probability density. Unfortunately, there is not a purely classical Hamiltonian description for systems in which particles are generated or annihilated. Therefore, the evolution equation for the density cannot be proposed as a direct extension of eq. (1.3). In fact, the terms which describe nonconservative processes must be explicitly derived from the dynamics of the single collision which takes place during each process.

The evolution of each density element ρ_n depends, in the first place, on the elastic interactions described by the Hamiltonian $\mathscr{H}_n$. The contribution of creation or annihilation events will add linear terms, in the form of operators acting on ρ_{n-1} and ρ_{n+1}, respectively, supposing that in each event only one particle is generated or destroyed. In general, the extended Liouville equation can be written as

$$\partial_t \rho_n = [\mathscr{H}_n, \rho_n] + (\partial_t \rho_n)_R \, , \quad (2.4)$$

where $(\partial_t \rho_n)_R$ describes the effects of nonconservative events. This term must be symmetric in its arguments. Furthermore, since the Hamiltonian term preserves the particle number, the conservation of probability implies

$$\int dx_1 \dots dx_n \, (\partial_t \rho_n)_R = \int dx_1 \dots dx_{n-1} (\partial_t \rho_{n-1})_R + \int dx_1 \dots dx_{n+1} (\partial_t \rho_{n+1})_R \, . \quad (2.5)$$

We shall explicitly consider here the four nonconservative events included in eq. (1.1):

a) Removal of a particle with coordinates x by interaction with the background gas. This process can be characterized by a transition frequency $\sigma_1(x)$, including the information about the distribution function of the background. It contributes to $(\partial_t \rho_n)_R$ with a gain term which depends lineary on ρ_{n+1}. Accordingly, a negative term must be added to take into account the loss of probability towards ρ_{n-1} by annihilation of a particle. Symmetrizing these terms in their arguments we obtain

$$(\partial_t \rho_n)_1 = (n+1) \int \mathrm{d}x\, \sigma_1(x) \rho_{n+1}(x_1 \ldots x_n x) - \rho_n(x_1 \ldots x_n) \sum_{i=1}^{n} \sigma_1(x_i)\,, \tag{2.6}$$

which indeed satisfy eq. (2.5). Eq. (2.6) is valid for $n \geq 1$: since no removal can occur in the absence of particles, the loss term must be eliminated for $n = 0$.

b) Creation of a particle with coordinates x by collision of a test particle in x' with the background. The colliding particle is scattered to coordinates x''. This process is characterized by a transition frequency $\sigma_2(x' \to xx'')$, which is a symmetric function in the pair of outgoing particles (x, x''). This transition probability also includes the information about the background gas. The positive gain term in $(\partial_t \rho_n)_R$ depends now on ρ_{n-1}. Symmetrization of the corresponding variables give the following terms, accomplishing the conservation of probability,

$$(\partial_t \rho_n)_2 = \frac{1}{n} \sum_{i,j}^{n}{}' \int \mathrm{d}x\, \sigma_2(x \to x_i x_j) \rho_{n-1}(x_1 \ldots \hat{x}_i \hat{x}_j \ldots x_n x) \\ - \rho_n(x_1 \ldots x_n) \int \mathrm{d}x\, \mathrm{d}x' \sum_{i=1}^{n} \sigma_2(x_i \to xx')\,. \tag{2.7}$$

The prime on the summation sign indicates that $i \neq j$. The hatted coordinates denote that those variables are missing in the arguments of ρ_{n-1}. For $n = 0$, $(\partial_t \rho_0)_2 = 0$.

c) Removal of a particle with coordinates x, by interaction with another particle in x', scattered by the collision to x''. It is characterized by a transition frequency $\sigma_3(xx' \to x'')$, which is symmetric in the coordinates of the ingoing particles (x, x'). Since it involves an annihilation, this process contributes to $(\partial_t \rho_n)_R$ from ρ_{n+1}, and the corresponding gain and loss terms read

$$(\partial_t \rho_n)_3 = (n+1) \sum_{i=1}^{n} \int \mathrm{d}x\, \mathrm{d}x'\, \sigma_3(xx' \to x_i) \rho_{n+1}(x_1 \ldots \hat{x}_i \ldots x_n xx') \\ - \rho_n(x_1 \ldots x_n) \sum_{i,j}^{n}{}' \int \mathrm{d}x\, \sigma_3(x_i x_j \to x)\,. \tag{2.8}$$

They also satisfy the probability conservation, eq. (2.5). Since two particles are required for the event to be produced, the loss term vanishes for $n = 0$ and $n = 1$; the gain term is also zero for $n = 0$.

d) Finally, creation of a particle with coordinates x'' by interaction of a pair in (x, y) which scatters to (x', y'). Its probability is given by a collision frequency $\sigma_4(xy \to x'y'x'')$, symmetric in the sets of variables (x, y) and (x', y', x''). The gain term depends on ρ_{n-1}, and symmetrization and conservation of probability determine

$$(\partial_t \rho_n)_4 = \frac{1}{n} \sum_{i,j,k}^{n}{}' \int \mathrm{d}x\, \mathrm{d}x'\, \sigma_4(xx' \to x_i x_j x_k) \rho_{n-1}(x_1 \ldots \hat{x}_i \hat{x}_j \hat{x}_k \ldots x_n x x') - \rho_n(x_1 \ldots x_n) \sum_{i,j}^{n}{}' \int \mathrm{d}x\, \mathrm{d}x'\, \mathrm{d}x''\, \sigma_4(x_i x_j \to xx'x'') . \tag{2.9}$$

The prime on the triple summation indicates that $i \neq j \neq k$. Now, the gain term vanishes for $n = 0, 1, 2$ and the loss term does the same for $n = 0, 1$.

Once having the explicit form of the temporal evolution that nonconservative processes determine for the density vector, we can proceed to study the effects of that evolution on the equations for the reduced distribution functions. In the next section, we develop the BBGKY hierarchy for the extended Liouville equation (2.4), when the described nonconservative events are taken into account. Then, the corresponding Boltzmann equations will be obtained to describe the evolution of the one-particle distribution function $f(\boldsymbol{x}, \boldsymbol{v}, t)$.

3. Extended BBGKY hierarchy and the Boltzmann equation

The evolution of the reduced distribution functions can be straightforwardly analyzed from their definition, eq. (2.3), and the dynamical law for the density vector, eq. (2.4). It is given by

$$\partial_t f_s(x_1 \ldots x_s, t) = \sum_{r=0}^{\infty} \frac{(s+r)!}{r!} \int \mathrm{d}x_{s+1} \ldots \mathrm{d}x_{s+r}\, \partial_t \rho_{s+r}(x_1 \ldots x_{s+r}) . \tag{3.1}$$

This equation contains two contributions, in accordance with the form of the right-hand side in eq. (2.4). In the first place, we note that the Hamiltonian term is linear in the probability density. Therefore, the original BBGKY hierarchy applies to each term in the summation of eq. (3.1), and the evolution law for the distribution functions can be written as

$$\partial_t f_s = [\mathcal{H}_s, f_s] + \int \mathrm{d}x_{s+1} \left[\sum_{i=1}^{s} V_{i\,s+1} \cdot f_{s+1} \right]$$
$$+ \sum_{r=0}^{\infty} \frac{(s+r)!}{r!} \int \mathrm{d}x_{s+1} \ldots \mathrm{d}x_{s+r} \, (\partial_t \rho_{s+r})_{\mathrm{R}} \, . \tag{3.2}$$

In this equation, the separation between elastic and nonconservative terms is evident. Furthermore, the form of the elastic contribution coincides with the original one, eq. (1.7). We shall therefore concentrate ourselves on the calculation of the expression for the nonconservative term,

$$(\partial_t f_s)_{\mathrm{R}} = \sum_{r=0}^{\infty} \frac{(s+r)!}{r!} \int \mathrm{d}x_{s+1} \ldots \mathrm{d}x_{s+r} \, (\partial_t \rho_{s+r})_{\mathrm{R}} \, . \tag{3.3}$$

This calculation must be explicitly done for each process considered in section 2, eqs. (2.6)–(2.9). The replacement and development of these equations in the right-hand side of eq. (3.3) is direct but highly tedious. Therefore, we only include here, as an example, the complete computation for the case of the creation of a particle by collision with the background [process (b), section 2]:

$$(\partial_t f_s)_2 = \sum_{r=0}^{\infty} \frac{(s+r)!}{r!} \int \mathrm{d}x_{s+1} \ldots \mathrm{d}x_{s+r} \, (\partial_t \rho_{s+r})_2$$
$$= \sum_{r=0}^{\infty} \frac{(s+r)!}{r!} \left[\int \mathrm{d}x_{s+1} \ldots \mathrm{d}x_{s+r} \frac{1}{s+r} \sum_{i,j}^{s+r}{}' \int \mathrm{d}x \, \sigma_2(x \to x_i x_j) \right.$$
$$\times \rho_{s+r-1}(x_1 \ldots \hat{x}_i \hat{x}_j \ldots x_{s+r} x)$$
$$\left. - \rho_{s+r}(x_1 \ldots x_{s+r}) \int \mathrm{d}x \, \mathrm{d}x' \sum_{i=1}^{s+r} \sigma_2(x_i \to x x') \right]$$
$$= \sum_{r=0}^{\infty} \frac{(s+r-1)!}{r!} \sum_{i,j}^{s}{}' \int \mathrm{d}x \, \sigma_2(x \to x_i x_j)$$
$$\times \int \mathrm{d}x_{s+1} \ldots \mathrm{d}x_{s+r} \, \rho_{s+r-1}(x_1 \ldots \hat{x}_i \hat{x}_j \ldots x_{s+r} x)$$
$$+ \sum_{r=1}^{\infty} \frac{(s+r-1)!}{(r-1)!} \sum_{i=1}^{s} \int \mathrm{d}x_{s+1} \ldots \mathrm{d}x_{s+r} \int \mathrm{d}x \, \sigma_2(x \to x_i x_{s+r})$$
$$\times \rho_{s+r-1}(x_1 \ldots \hat{x}_i \ldots x_{s+r-1} x)$$
$$+ \sum_{r=1}^{\infty} \frac{(s+r-1)!}{(r-1)!} \sum_{j=1}^{s} \int \mathrm{d}x_{s+1} \ldots \mathrm{d}x_{s+r} \int \mathrm{d}x \, \sigma_2(x \to x_{s+r} x_j)$$
$$\times \rho_{s+r-1}(x_1 \ldots \hat{x}_j \ldots x_{s+r-1} x)$$

$$+\sum_{r=2}^{\infty}\frac{(s+r-1)!}{(r-2)!}\int dx_{s+1}\ldots dx_{s+r}\int dx\,\sigma_2(x\to x_{s+1}x_{s+r})$$
$$\times\,\rho_{s+r-1}(x_1\ldots\hat{x}_{s+1}\ldots x_{s+r-1}x)$$
$$-\sum_{r=0}^{\infty}\frac{(s+r)!}{r!}\sum_{i=1}^{s}\int dx\,dx'\,\sigma_2(x_i\to xx')$$
$$\times\int dx_{s+1}\ldots dx_{s+r}\,\rho_{s+r}(x_1\ldots x_{s+r})$$
$$-\sum_{r=1}^{\infty}\frac{(s+r)!}{(r-1)!}\int dx_{s+1}\ldots dx_{s+r}\int dx\,dx'\,\sigma_2(x_{s+1}\to xx')$$
$$\times\,\rho_{s+r}(x_1\ldots x_{s+r})\,. \tag{3.4}$$

A redefinition of the summation indices enables the reconstruction of the distribution functions to give

$$(\partial_t f_s)_2=\sum_{i,j}^{s}{}'\int dx\,\sigma_2(x\to x_ix_j)f_{s-1}(x_1\ldots\hat{x}_i\hat{x}_j\ldots x_sx)$$
$$+2\sum_{i=1}^{s}\int dx\,dx'\,\sigma_2(x\to x_ix')f_s(x_1\ldots\hat{x}_i\ldots x_sx)$$
$$-f_s(x_1\ldots x_s)\sum_{i=1}^{s}\int dx\,dx'\,\sigma_2(x_i\to xx')\,. \tag{3.5}$$

In the same way, the contributions to the evolution of the reduced distributions can be calculated for any nonconservative process, giving

$$(\partial_t f_s)_1=-\,f_s(x_1\ldots x_s)\sum_{i=1}^{s}\sigma_1(x_i)\,, \tag{3.6a}$$

$$(\partial_t f_s)_2=\sum_{i,j}^{s}{}'\int dx\,\sigma_2(x\to x_ix_j)f_{s-1}(x_1\ldots\hat{x}_i\hat{x}_j\ldots x_sx)$$
$$+2\sum_{i=1}^{s}\int dx\,dx'\,\sigma_2(x\to x_ix')f_s(x_1\ldots\hat{x}_i\ldots x_sx)$$
$$-\,f_s(x_1\ldots x_s)\sum_{i=1}^{s}\int dx\,dx'\,\sigma_2(x_i\to xx')\,, \tag{3.6b}$$

$$(\partial_t f_s)_3=\sum_{i=1}^{s}{}'\int dx\,dx'\,\sigma_3(xx'\to x_i)f_{s+1}(x_1\ldots\hat{x}_i\ldots x_sxx')$$
$$-2\sum_{i=1}^{s}\int dx\,dx'\,\sigma_3(x_ix'\to x)f_{s+1}(x_1\ldots x_sx')$$
$$-\,f_s(x_1\ldots x_s)\sum_{i,j}^{s}{}'\int dx\,\sigma_3(x_ix_j\to x)\,, \tag{3.6c}$$

$$(\partial_t f_s)_4 = \sum_{ijk}^{s}{}' \int \mathrm{d}x\, \mathrm{d}x'\, \sigma_4(xx' \to x_i x_j x_k) f_{s-1}(x_1 \ldots \hat{x}_i \hat{x}_j \hat{x}_k \ldots x_s x x')$$
$$+ 3 \sum_{i,j}^{s}{}' \int \mathrm{d}x\, \mathrm{d}x'\, \mathrm{d}x''\, \sigma_4(xx' \to x_i x_j x'') f_s(x_1 \ldots \hat{x}_i \hat{x}_j \ldots x_s x x')$$
$$+ 3 \sum_{i=1}^{s} \int \mathrm{d}x\, \mathrm{d}x'\, \mathrm{d}x''\, \mathrm{d}y\, \sigma_4(xx' \to x_i x'' y) f_{s+1}(x_1 \ldots \hat{x}_i \ldots x_s x x')$$
$$- 2 \sum_{i=1}^{s} \int \mathrm{d}x\, \mathrm{d}x'\, \mathrm{d}x''\, \mathrm{d}y\, \sigma_4(x_i y \to x x' x'') f_{s+1}(x_1 \ldots x_s x y)$$
$$- f_s(x_1 \ldots x_s) \sum_{i,j}^{s}{}' \int \mathrm{d}x\, \mathrm{d}x'\, \mathrm{d}x''\, \sigma_4(x_i x_j \to x x' x'') . \qquad (3.6\mathrm{d})$$

Eqs. (3.6) constitute the BBGKY hierarchy for the creation and removal events here considered.

The contribution of the nonconservative processes to the Boltzmann equation is obtained evaluating the BBGKY formulae for $s = 1$, and applying the hypothesis of molecular chaos, eq. (1.8). Calling $f \equiv f_1$, we find

$$(\partial_t f)_1 = -f(x_1)\sigma_1(x_1) , \qquad (3.7\mathrm{a})$$

$$(\partial_t f)_2 = 2 \int \mathrm{d}x\, \mathrm{d}x'\, \sigma_2(x \to x_1 x') f(x) - f(x_1) \int \mathrm{d}x\, \mathrm{d}x'\, \sigma_2(x_1 \to x x') , \qquad (3.7\mathrm{b})$$

$$(\partial_t f)_3 = \int \mathrm{d}x\, \mathrm{d}x'\, \sigma_3(xx' \to x_1) f(x) f(x')$$
$$- 2 f(x_1) \int \mathrm{d}x\, \mathrm{d}x'\, \sigma_3(x_1 x' \to x) f(x') , \qquad (3.7\mathrm{c})$$

$$(\partial_t f)_4 = 3 \int \mathrm{d}x\, \mathrm{d}x'\, \mathrm{d}x''\, \mathrm{d}y\, \sigma_4(xx' \to x_1 x'' y) f(x) f(x')$$
$$- 2 f(x_1) \int \mathrm{d}x\, \mathrm{d}x'\, \mathrm{d}x''\, \mathrm{d}y\, \sigma_4(x_1 y \to x x' x'') f(y) . \qquad (3.7\mathrm{d})$$

These terms must be added to the usual collision integral in eq. (1.9).

It is possible to identify in each contribution to $(\partial_t f)_R$ the elementary process from which any term of eqs. (3.7) arises. In eq. (3.7a) the only contribution represents a loss to the distribution function due to the removal of a particle in x_1, with probability $\sigma_1(x_1)$. The loss term in eq. (3.7b) identifies the collision $(x_1) \to (x, x')$, which creates a new particle and modifies the coordinates of the incoming particle. On the other hand, the gain term represents the processes $(x) \to (x_1, x')$ and $(x') \to (x_1, x)$, which have the same contribution. In the same way, in eq. (3.7c) the equivalent collisions $(x_1, x') \to (x)$ and $(x_1, x) \to (x')$ determine a loss for the distribution function and $(x, x') \to (x_1)$ is a positive contribution. Finally, in eq. (3.7d) the loss and gain terms are given by $(x_1, y) \to (x, x', x'')$ and $(x, x') \to (x_1, x'', y)$ respectively. The equivalent processes determine the prefactors of each term.

At this point, we have reached the main aim of this paper, that is, the obtainment of the extended Boltzmann equation from the Liouville equation through the construction of a BBGKY hierarchy. Now, it is necessary to compare it with the previously proposed models, in order to understand eventual involved assumptions.

4. Comparison with the model Boltzmann equation (1.1)

The main difference between the nonconservative contributions to the Boltzmann equation calculated in section 3, eqs. (3.7), and the model equation (1.1) consists in the fact that, in this last case, each creation or removal effect determines the addition of only one term to the collision integral. This additional term is positive for creation events and negative for removal processes. Instead, from the BBGKY hierarchy, we obtained in general a gain and a loss contribution to the right-hand side of the Boltzmann equation. As we discussed in section 3, the negative contribution in a creation process has its origin in the scattering of the incoming particles, which determines a loss of probability in the coordinates of those particles, even when a new particle is created. On the other hand, when a particle is destroyed by collision with another particle [process (c), section 2], the scattering determines that the remaining particle positively contributes to the distribution function in its new coordinates.

Therefore, the difference between both formulations lies in the scattering process taking place when a particle is generated or annihilated. Indeed, even when it is not explicitly said in the proposed model Boltzmann equation (1.1), the colliding molecules are not supposed to be scattered during the creation and removal events. Instead, the nonconservative processes formulation here introduced consider the possibility of such scattering.

It is then interesting to analyze the form of the transition frequencies σ_i, defined in section 2, which enables the derivation of the Boltzmann equation (1.1) from the nonconservative contributions computed in section 3, eqs. (3.7). These transition frequencies must determine the coordinates of the outgoing colliding particles to be equal to those of the incoming molecules. On the other hand, they must satisfy the symmetry properties described in section 2.

Furthermore, an exact identification between both formulations requires the background distribution function $g(\boldsymbol{v})$ to be made explicit in the collision frequencies describing the interaction with the host medium. The relation between the velocity variables and the phase space coordinates is straightforward, since the collision frequencies are not expected to depend on the spatial variables.

The imposed conditions meet in the following forms for the transition probabilities:

$$\sigma_1(x) = \int \mathrm{d}z \, \sigma_{\mathrm{B}}^{\mathrm{r}}(xz) g(z) \,, \tag{4.1a}$$

$$\sigma_2(x' \to xx'') = \frac{1}{2}\left[\delta(x - x') \int \mathrm{d}z \, \sigma_{\mathrm{B}}^{\mathrm{c}}(xz \to x'') g(z) \right.$$
$$\left. + \, \delta(x'' - x') \int \mathrm{d}z \, \sigma_{\mathrm{B}}^{\mathrm{c}}(x''z \to x) g(z) \right] , \tag{4.1b}$$

$$\sigma_3(x'x'' \to x) = \tfrac{1}{2}[\delta(x - x')\sigma^{\mathrm{r}}(x'x'') + \delta(x - x'')\sigma^{\mathrm{r}}(x''x')] \,, \tag{4.1c}$$

$$\sigma_4(x'x'' \to xyy') = \tfrac{1}{6}[\delta(x' - y)\delta(x'' - y')\sigma^{\mathrm{c}}(x'x'' \to x)$$
$$+ \, \delta(x' - y')\delta(x'' - y)\sigma^{\mathrm{c}}(x'x'' \to x) + \delta(x' - x)\delta(x'' - y)\sigma^{\mathrm{c}}(x'x'' \to y'')$$
$$+ \, \delta(x' - y)\delta(x'' - x)\sigma^{\mathrm{c}}(x'x'' \to y') + \delta(x' - x)\delta(x'' - y')\sigma^{\mathrm{c}}(x'x'' \to y)$$
$$+ \, \delta(x' - y')\delta(x'' - x)\sigma^{\mathrm{c}}(x'x'' \to y)] \,. \tag{4.1d}$$

The replacement of these particular forms in eqs. (3.7) completely identifies both formulations for the extended kinetic theory.

5. Conclusion

The extended kinetic theory, in which generation and annihilation of particles are taken into account, is formulated by means of a generalized Boltzmann equation. Up to this moment, the form of this generalized equation had been heuristically proposed, involving an *ad hoc* construction of the corresponding collision terms.

In this paper, we have developed a formal derivation of the extended kinetic equation from the Liouville theorem, which governs the evolution of the probability density in the phase space. This derivation has required a generalization of the definition of the probability density and the reduced distribution functions, since the number of particles is not a constant in the system. In fact, we have introduced a density vector whose components describe the conditional probability density in the phase space, for a given number of particles. The reduced distribution functions were accordingly redefined, in order to preserve their underlying concept.

The nonconservative processes have been introduced in the Liouville equation by analyzing the effects that these microscopic events produce in the variation of the probability density. When applied to the evolution equations for the reduced distributions, the extended Liouville theorem has given ground to an extended BBGKY hierarchy. It is interesting to note that, in this generalized hierarchy, the reduced s-particle distribution is not only coupled with the $(s+1)$-particle distribution, as occurs in the original equations, but also with the $(s-1)$-particle distribution. This is a direct consequence of the existence of creation processes.

Through the hypothesis of molecular chaos, the last step of the extended BBGKY hierarchy determines the form of the generalized Boltzmann equation. It is found to differ from the previously proposed models. The origin of the difference is due to the fact that in the previous models the particles which interact during a generation or annihilation event are not supposed to be scattered. This assumption has been removed in our analysis, giving place to gain and loss terms which explicitly reduce to the previous models when the transition frequencies inhibit the scattering.

Through this generalized BBGKY hierarchy, a new class of model Boltzmann equations describing nonconservative processes has arisen. The study of their solutions will be the subject of future work.

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