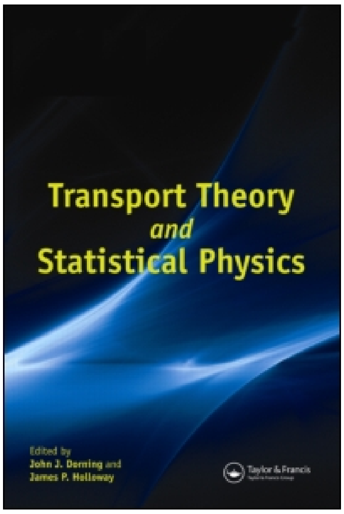

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SOME NEW PROPERTIES OF THE KINETIC EQUATION FOR THE CONSISTENT BOLTZMANN ALGORITHM

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ABSTRACT

We study properties of the consistent Boltzmann algorithm for dense gases, using its limiting kinetic equation. First, we derive an *H*-theorem for this equation. Then, following the classical derivation by Chapman and Cowling, we find approximations to the equations of continuity, momentum, and energy. The first order correction terms with respect to the particle diameter turn out to be the same as for the Enskog equation. These results confirm previous derivations, based on the virial, of the corresponding equation of state.

Key Words: Kinetic theory; Direct simulation Monte Carlo; Consistent Boltzmann algorithm; Dense gases; H-theorem

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1. INTRODUCTION

Direct Simulation Monte Carlo (DSMC) is presently the most widely used numerical algorithm in kinetic theory.[5] In this method, a system of simulation particles

$$(x_i(t), v_i(t)), \quad i = 1, \ldots, N, \quad t \geq 0,$$

is used to approximate the behaviour of the real gas. Independent motion (free flow) of the particles and their pairwise interactions (collisions) are separated using a splitting procedure. During the free flow step, particles are moved according to their velocities,

$$x_i(t + \Delta t) = x_i(t) + \int_t^{t+\Delta t} v_i(s)\, ds,$$

and boundary conditions are taken into account. During the collision step, particle pairs $(x, v), (y, w)$ are randomly chosen in small cells of the position space, according to the collision probability for the interparticle potential. The post-collision velocities

$$v^* = v + e\,(e, w - v)\,, \qquad w^* = w - e\,(e, w - v) \tag{1.1}$$

are determined by randomly selecting a direction vector e from the unit sphere $\mathcal{S}^2 \subset \mathcal{R}^3$. Here $(\cdot\,,\cdot)$ denotes the scalar product in $\mathcal{R}^3$. The number of collisions at each time step Δt is computed from the local collision frequency.

Recently, the Consistent Boltzmann Algorithm (CBA) was introduced as a simple variant of DSMC for dense gases.[1] The main advantages of CBA over Enskog-based schemes (see Refs. [8,12]) are its simplicity in implementation and almost negligible effect on computational efficiency for a standard DSMC program. Transport properties are in good agreement with molecular dynamics data even at high density.[2] Besides the standard problems in kinetic theory, CBA has proved useful in the study of granular materials[10] and nuclear physics.[11,13]

Although CBA can be generalized to other potentials,[2] here we will only consider the hard sphere gas with particle diameter σ. In CBA the collision process is as in DSMC with two modifications. First, when a pair collides each particle is displaced a distance σ into the direction

e or $-e$ (cf. Eq. (1.1)), i.e.,

$$x^* = x + \sigma \frac{(v^* - w^*) - (v - w)}{\|(v^* - w^*) - (v - w)\|}, \qquad y^* = y - \sigma \frac{(v^* - w^*) - (v - w)}{\|(v^* - w^*) - (v - w)\|}, \tag{1.2}$$

where $\|\cdot\|$ denotes the Euclidean norm in $\mathcal{R}^3$. Second, the dense hard sphere collision frequency, which contains a factor χ depending on the local density, is used. The function χ is equal to unity for a rarefied gas, and increases with increasing density, becoming infinity as the gas approaches the state of close-packing. Approximations to its value may be found in Ref. [7, Ch. 16.21].

A theoretical foundation of this variant of DSMC has been established in Ref. [9] by deriving the limiting (as $N \to \infty$) **kinetic equation of CBA**,

$$\frac{\partial}{\partial t} p(t,x,v) + (v, \nabla_x) p(t,x,v) = \int_{\mathcal{R}^3} dw \int_{\mathcal{S}^2} de B(v,w,e) \times [\chi(\varrho(t,x^*)) p(t,x^*,v^*) p(t,x^*,w^*) - \chi(\varrho(t,x)) p(t,x,v) p(t,x,w)], \tag{1.3}$$

where p is the one-particle distribution function, B denotes the collision kernel, and

$$\varrho(t,x) = \int_{\mathcal{R}^3} p(t,x,v)\, dv$$

is the density. Note that, in the case $\chi \equiv 1$, $\sigma = 0$, Eq. (1.3) reduces to the **Boltzmann equation**

$$\frac{\partial}{\partial t} p(t,x,v) + (v, \nabla_x) p(t,x,v) = \int_{\mathcal{R}^3} dw \int_{\mathcal{S}^2} de B(v,w,e) [p(t,x,v^*) p(t,x,w^*) - p(t,x,v) p(t,x,w)].$$

The purpose of this paper is to study some properties of Eq. (1.3) in relation to corresponding properties of the **Enskog equation** (cf. Ref. [7, Ch. 16.3])

$$\frac{\partial}{\partial t} f(t,x,v) + (v, \nabla_x) f(t,x,v) = \int_{\mathcal{R}^3} dw \int_{\mathcal{S}^2_+} de\, \sigma^2 (e, w - v) \Big[\chi(\varrho(t, x + \frac{1}{2}\sigma e)) f(t,x,v^*) f(t, x + \sigma e, w^*) - \chi(\varrho(t, x - \frac{1}{2}\sigma e)) f(t,x,v) f(t, x - \sigma e, w)\Big]. \tag{1.4}$$

Here f is the one-particle number density function, and the notations

$$\mathcal{S}^2_+ = \mathcal{S}^2_+(v,w) = \{e : (e, w-v) > 0\}, \qquad \mathcal{S}^2_- = \{e : (e, w-v) < 0\} \tag{1.5}$$

are used. Taking into account Eqs. (1.1), (1.2), and the hard sphere collision kernel, Eq. (1.3) takes the form

$$\begin{aligned} &\frac{\partial}{\partial t} f(t,x,v) + (v, \nabla_x) f(t,x,v) \\ &\quad = \int_{\mathcal{R}^3} dw \int_{\mathcal{S}^2_+} de\, \sigma^2 (e, w-v) \Big[\chi(\varrho(t, x+\sigma e)) f(t, x+\sigma e, v^*) \\ &\qquad \times f(t, x+\sigma e, w^*) - \chi(\varrho(t,x)) f(t,x,v) f(t,x,w) \Big]. \end{aligned} \tag{1.6}$$

In Sec. 2, following ideas from Ref. [14] for the Enskog equation, we derive an H-theorem. In the Enskog case, such result turned out to be useful for studying the existence problem and the trend to equilibrium (see, e.g., Refs. [3,4]). In Sec. 3, following the classical derivation by Chapman and Cowling, Ref. [7, Ch. 16], we find approximations to the equations of continuity, momentum and energy. The first order correction terms with respect to the particle diameter turn out to be the same as for the Enskog equation. These results confirm previous derivations, based on the virial, of the corresponding equation of state.[1]

2. *H*-THEOREM

According to Eq. (1.1), the displacements Eq. (1.2) take the form

$$x^* = x + \psi(v,w,e), \qquad y^* = y - \psi(v,w,e),$$

where the notation

$$\psi(v,w,e) = \sigma\, e\, \mathrm{sign}(e, w-v)$$

is used. Note that

$$\psi(v^*, w^*, e) = -\psi(v,w,e) = \psi(w,v,e) \tag{2.1}$$

and

$$B(v,w,e) = B(v^*, w^*, e) = B(w,v,e) = B(v,w,-e), \tag{2.2}$$

for $B(v, w, e) = \text{const}\,|(e, w - v)|$. Using Eqs. (2.1), (2.2), one obtains

$$\begin{aligned}
&\int_{\mathcal{R}^3} dx \int_{\mathcal{R}^3} dv \int_{\mathcal{R}^3} dw \int_{\mathcal{S}^2} de\, \varphi(x, v)\, B(v, w, e)\, \chi(\varrho(t, x^*))\, p(t, x^*, v^*)\, p(t, x^*, w^*) \\
&\quad = \int_{\mathcal{R}^3} dx \int_{\mathcal{R}^3} dv \int_{\mathcal{R}^3} dw \int_{\mathcal{S}^2} de \\
&\quad \times \varphi(x - \psi(v, w, e), v)\, B(v, w, e)\, \chi(\varrho(t, x))\, p(t, x, v^*)\, p(t, x, w^*) \\
&\quad = \int_{\mathcal{R}^3} dx \int_{\mathcal{R}^3} dv \int_{\mathcal{R}^3} dw \int_{\mathcal{S}^2} de\, \varphi(x^*, v^*)\, B(v, w, e)\, \chi(\varrho(t, x))\, p(t, x, v)\, p(t, x, w).
\end{aligned}$$

Thus, the weak form of Eq. (1.3) is

$$\begin{aligned}
&\frac{d}{dt} \int_{\mathcal{R}^3 \times \mathcal{R}^3} \varphi(x, v)\, p(t, x, v)\, dx\, dv \\
&\quad = \int_{\mathcal{R}^3 \times \mathcal{R}^3} (v, (\nabla_x \varphi)(x, v))\, p(t, x, v)\, dx\, dv + \int_{\mathcal{R}^3} dx \int_{\mathcal{R}^3} dv \int_{\mathcal{R}^3} dw \int_{\mathcal{S}^2} de \\
&\quad \times \chi(\varrho(t, x))\, B(v, w, e) \Big[\varphi(x^*, v^*) - \varphi(x, v)\Big] p(t, x, v)\, p(t, x, w),
\end{aligned}$$

or, equivalently,

$$\begin{aligned}
&\frac{d}{dt} \int_{\mathcal{R}^3 \times \mathcal{R}^3} \varphi(x, v)\, p(t, x, v)\, dx\, dv \\
&\quad = \int_{\mathcal{R}^3 \times \mathcal{R}^3} (v, (\nabla_x \varphi)(x, v))\, p(t, x, v)\, dx\, dv + \frac{1}{2} \int_{\mathcal{R}^3} dx \int_{\mathcal{R}^3} dv \int_{\mathcal{R}^3} dw \int_{\mathcal{S}^2} de \\
&\quad \times \chi(\varrho(t, x))\, B(v, w, e) \Big[\varphi(x + \psi(v, w, e), v^*) + \varphi(x - \psi(v, w, e), w^*) \\
&\quad - \varphi(x, v) - \varphi(x, w)\Big] p(t, x, v)\, p(t, x, w). \qquad (2.3)
\end{aligned}$$

The form (2.3) is convenient for deriving an H-theorem. We consider

$$\varphi(x, v) = \log p(t, x, v)$$

and

$$H(t) = \int_{\mathcal{R}^3} \int_{\mathcal{R}^3} p(t, x, v)\, \log p(t, x, v)\, dv\, dx.$$

Note that

$$\int_{\mathcal{R}^3\times\mathcal{R}^3} (v, \nabla_x \log p(t,x,v))\, p(t,x,v)\, dx\, dv = \int_{\mathcal{R}^3\times\mathcal{R}^3} \frac{(v, \nabla_x p(t,x,v))}{p(t,x,v)}\, p(t,x,v)\, dx\, dv = 0.$$

Using the elementary inequality

$$a(\log b - \log a) \le b - a, \quad a, b > 0,$$

one obtains

$$\begin{aligned}
\frac{d}{dt} H(t) =& \frac{1}{2}\int_{\mathcal{R}^3} dx \int_{\mathcal{R}^3} dv \int_{\mathcal{R}^3} dw \int_{\mathcal{S}^2} de\, \chi(\varrho(t,x))\, B(v,w,e) \\
&\times \Big\{ \log\Big[p(t,x+\psi(v,w,e),v^*)\, p(t,x-\psi(v,w,e),w^*)\Big] \\
&- \log\Big[p(t,x,v)\,p(t,x,w)\Big]\Big\}\, p(t,x,v)\,p(t,x,w) \\
\le& \frac{1}{2}\int_{\mathcal{R}^3} dx \int_{\mathcal{R}^3} dv \int_{\mathcal{R}^3} dw \int_{\mathcal{S}^2} de\, \chi(\varrho(t,x))\, B(v,w,e) \\
&\times \Big[p(t,x+\psi(v,w,e),v^*)\,p(t,x-\psi(v,w,e),w^*) - p(t,x,v)\,p(t,x,w)\Big] \\
=& \frac{1}{2}\int_{\mathcal{R}^3} dx \int_{\mathcal{R}^3} dv \int_{\mathcal{R}^3} dw \int_{\mathcal{S}^2} de\, \chi(\varrho(t,x))\, B(v,w,e) \\
&\times \Big[p(t,x-\psi(v,w,e),v)\,p(t,x+\psi(v,w,e),w) - p(t,x,v)\,p(t,x,w)\Big] \\
=:& I(t).
\end{aligned}$$

With the notations (1.5), the correction functional takes the form

$$\begin{aligned}
I(t) &= \int_{\mathcal{R}^3} dx \int_{\mathcal{R}^3} dv \int_{\mathcal{R}^3} dw \int_{\mathcal{S}^2_+(v,w)} de\, \chi(\varrho(t,x))\, B(v,w,e) \\
&\quad \times \Big[p(t,x-\psi(v,w,e),v)\,p(t,x+\psi(v,w,e),w) - p(t,x,v)\,p(t,x,w)\Big] \\
&= \int_{\mathcal{R}^3} dx \int_{\mathcal{R}^3} dv \int_{\mathcal{R}^3} dw \int_{\mathcal{S}^2_-(v,w)} de\, \chi(\varrho(t,x))\, B(v,w,e) \\
&\quad \times \Big[p(t,x-\psi(v,w,e),v)\,p(t,x+\psi(v,w,e),w) - p(t,x,v)\,p(t,x,w)\Big] \\
&= \int_{\mathcal{R}^3} dx \int_{\mathcal{R}^3} dv \int_{\mathcal{R}^3} dw \int_{\mathcal{S}^2_+(v,w)} de\, \chi(\varrho(t,x))\, B(v,w,e) \\
&\quad \times \Big[p(t,x-\sigma e,v)\,p(t,x+\sigma e,w) - p(t,x,v)\,p(t,x,w)\Big].
\end{aligned}$$

Introducing the functional

$$\tilde{H}(t) = H(t) - \int_0^t I(s)\, ds,$$

one obtains

$$\frac{d}{dt}\,\tilde{H}(t) \leq 0.$$

Note that, in the Boltzmann case $\sigma = 0$, one obtains $I(t) = 0$.

A similar functional has been suggested in Ref. [14] in the case of the Enskog Eq. (1.4). It was proved in Ref. [4] that this counterpart of the Boltzmann H-functional decreases for global solutions which are known to exist for small data. This result was used in Ref. [3] for studying the trend to equilibrium.

3. EQUATIONS OF CONTINUITY, MOMENTUM, AND ENERGY

With the short-hand notations

$$f(x) = f(t,x,v)\,, \qquad f_1(x) = f(t,x,v_1)\,,$$
$$f^*(x) = f(t,x,v^*), \qquad f_1^*(x) = f(t,x,v_1^*),$$

and $v \cdot w = (v,w)$, Eq. (1.6) takes the form

$$\left[\frac{\partial}{\partial t} + v \cdot \nabla_x\right] f = \int\int \Big[f^*(x+\sigma e) f_1^*(x+\sigma e) - f(x) f_1(x)\Big]\, \sigma^2 c(v_1 - v)\cdot e\, de\, dv_1. \tag{3.1}$$

Here integration de is over $\mathcal{S}_+^2(v, v_1)$ (cf. Eq. (1.5)) and integration dv_1 is over $\mathcal{R}^3$. For simplicity we set $\chi \equiv 1$. The uniform steady state is

$$f^{(0)} = n\Big(\frac{m}{2\pi kT}\Big)^{3/2} \exp\Big(-\frac{m\|v - c_0\|^2}{2kT}\Big). \tag{3.2}$$

A first approximation to the solution of Eq. (3.1) is $f = f^{(0)}$, a second approximation is

$$f^{(1)} = f^{(0)}(1 + \Phi^{(1)}), \tag{3.3}$$

where $\Phi^{(1)}$ is a linear function of the first derivatives of number density n, temperature T, and mass velocity c_0. In the following derivations we neglect all products of derivatives and derivatives of higher order (cf. Ref. [7, Ch. 16]).

3.1. Left-Hand Side of the Kinetic Equation

Consider the left-hand side of Eq. (3.1):

$$\left[\frac{\partial}{\partial t} + v \cdot \nabla_x\right] f^{(1)} = \left[\frac{\partial}{\partial t} + v \cdot \nabla_x\right] f^{(0)} = f^{(0)}\left[\frac{\partial}{\partial t} + v \cdot \nabla_x\right] \log f^{(0)}.$$

Note that

$$\frac{\partial}{\partial t} \log f^{(0)} = \frac{1}{n}\frac{\partial}{\partial t} n - \frac{3}{2T}\frac{\partial}{\partial t} T + \frac{m}{2kT^2}\frac{\partial}{\partial t} T \, \|v - c_0\|^2 + \frac{m}{kT}(v - c_0)\frac{\partial}{\partial t} c_0$$

and

$$\nabla_x \log f^{(0)} = \frac{1}{n}\nabla_x n - \frac{3}{2T}\nabla_x T + \frac{m}{2kT^2}\nabla_x T \, \|v - c_0\|^2 + \frac{m}{kT}(\nabla_x c_0)(v - c_0).$$

Multiplying with $\psi = 1$ and integrating with respect to v, one obtains

$$\int dv f^{(0)} \frac{\partial}{\partial t} \log f^{(0)} = \frac{\partial}{\partial t} n - \frac{3n}{2T}\frac{\partial}{\partial t} T + \frac{3n}{2T}\frac{\partial}{\partial t} T$$

and

$$\begin{aligned} &\int dv f^{(0)} v \cdot \nabla_x \log f^{(0)} \\ &\quad = c_0 \cdot \nabla_x n - \frac{3n}{2T} c_0 \cdot \nabla_x T + \frac{mn}{2kT^2} c_0 \cdot \nabla_x T \, \frac{3kT}{m} + n \,\mathrm{div}(c_0) \\ &\quad = c_0 \cdot \nabla_x n + n \,\mathrm{div}(c_0). \end{aligned}$$

Finally,

$$\int dv f^{(0)} \left[\frac{\partial}{\partial t} + v \cdot \nabla_x\right] \log f^{(0)} = \frac{D}{Dt} n + n \,\mathrm{div}(c_0) \tag{3.4}$$

where

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + c_0 \cdot \nabla_x. \tag{3.5}$$

Multiplying with $\psi = v - c_0$ and integrating with respect to v, one obtains (cf. Eq. (A.2))

$$\int dv\,(v-c_0)f^{(0)}\,\frac{\partial}{\partial t}\log f^{(0)} = n\,\frac{\partial}{\partial t}\,c_0$$

and (cf. Eqs. (A.2), (A.4), (A.3))

$$\begin{aligned}
&\int dv\,(v-c_0)f^{(0)}\,v\cdot\nabla_x\log f^{(0)} \\
&= \frac{kT}{m}\nabla_x n - \frac{3kn}{2m}\nabla_x T + \frac{m}{2kT^2}\int dv\,(v-c_0)f^{(0)}\,(v-c_0)\cdot\nabla_x T\,\|v-c_0\|^2 \\
&\quad + \frac{m}{kT}\int dv\,(v-c_0)f^{(0)}\,(v-c_0)\cdot(\nabla_x c_0)(v-c_0) \\
&\quad + \frac{m}{kT}\int dv\,(v-c_0)f^{(0)}\,c_0(\nabla_x c_0)(v-c_0) \\
&= \frac{kT}{m}\nabla_x n - \frac{3kn}{2m}\nabla_x T + \frac{m}{2kT^2}5n\left(\frac{kT}{m}\right)^2\nabla_x T + \frac{m}{kT}\,\frac{kTn}{m}\,c_0(\nabla_x c_0) \\
&= \frac{kT}{m}\nabla_x n + \frac{nk}{m}\nabla_x T + n(c_0\cdot\nabla_x)c_0.
\end{aligned}$$

Note that $\nabla_x c_0$ is a matrix, $\left((\partial/\partial x_i)\,c_{0,j}\right)_{i,j=1}^3$ and

$$[c_0(\nabla_x c_0)]_i = c_{0,1}\,\frac{\partial}{\partial x_1}\,c_{0,i} + c_{0,2}\,\frac{\partial}{\partial x_2}\,c_{0,i} + c_{0,3}\,\frac{\partial}{\partial x_3}\,c_{0,i} = (c_0\cdot\nabla_x)c_{0,i}.$$

Finally one obtains (cf. Eq. (3.5))

$$\begin{aligned}
&\int dv\,(v-c_0)f^{(0)}\left[\frac{\partial}{\partial t} + v\cdot\nabla_x\right]\log f^{(0)} \\
&= n\,\frac{\partial}{\partial t}\,c_0 + n(c_0\cdot\nabla_x)c_0 + \frac{kT}{m}\nabla_x n + \frac{nk}{m}\nabla_x T = n\,\frac{D}{Dt}\,c_0 + \frac{1}{m}\nabla_x(k\,nT).
\end{aligned} \tag{3.6}$$

Multiplying with $\psi = \|v - c_0\|^2$ and integrating with respect to v, one obtains (cf. Eq. (A.5))

$$\begin{aligned}
&\int dv\,\|v-c_0\|^2 f^{(0)}\,\frac{\partial}{\partial t}\log f^{(0)} \\
&= \frac{\partial}{\partial t}\,n\,\frac{3kT}{m} - \frac{3}{2T}\,\frac{\partial}{\partial t}\,Tn\,\frac{3kT}{m} + \frac{m}{2kT^2}\,\frac{\partial}{\partial t}\,T15n\left(\frac{kT}{m}\right)^2 \\
&= \frac{3kT}{m}\,\frac{\partial}{\partial t}\,n - \frac{9kn}{2m}\,\frac{\partial}{\partial t}\,T + \frac{15kn}{2m}\,\frac{\partial}{\partial t}\,T = \frac{3kT}{m}\,\frac{\partial}{\partial t}\,n + \frac{3kn}{m}\,\frac{\partial}{\partial t}\,T
\end{aligned}$$

and (cf. Eqs. (A.5), (A.6))

$$\begin{aligned}
&\int dv\,\|v-c_0\|^2 f^{(0)}\, v\cdot\nabla_x \log f^{(0)} \\
&= \frac{3kT}{m}\, c_0\cdot\nabla_x n - \frac{9kn}{2m}\, c_0\cdot\nabla_x T + \frac{m}{2kT^2}\, c_0\cdot\nabla_x T 15n\left(\frac{kT}{m}\right)^2 \\
&\quad + \frac{m}{kT}\int dv\,\|v-c_0\|^2 f^{(0)}\,(v-c_0)\cdot(\nabla_x c_0)(v-c_0) \\
&= \frac{3kT}{m}\, c_0\cdot\nabla_x n - \frac{9kn}{2m}\, c_0\cdot\nabla_x T + \frac{15nk}{2m}\, c_0\cdot\nabla_x T + \frac{m}{kT}\, 5n\left(\frac{kT}{m}\right)^2 \operatorname{div}(c_0) \\
&= \frac{3kT}{m}\, c_0\cdot\nabla_x n + \frac{3kn}{m}\, c_0\cdot\nabla_x T + \frac{5nkT}{m}\operatorname{div}(c_0).
\end{aligned}$$

Finally one obtains (cf. Eq. (3.5))

$$\begin{aligned}
&\int dv\,\|v-c_0\|^2 f^{(0)}\left[\frac{\partial}{\partial t} + v\cdot\nabla_x\right]\log f^{(0)} \\
&\quad = \frac{3kT}{m}\frac{D}{Dt}\, n + \frac{3kn}{m}\frac{D}{Dt}\, T + \frac{5nkT}{m}\operatorname{div}(c_0).
\end{aligned} \tag{3.7}$$

3.2. Right-Hand Side of the Kinetic Equation

Consider the term in brackets at the right-hand side of Eq. (3.1). Expanding f_1, f_1^* by Taylor's theorem, and retaining only the first derivatives, gives

$$(f^* f_1^* - f f_1) + \sigma e\cdot(f^*\,\nabla_x f_1^* + f_1^*\,\nabla_x f^*). \tag{3.8}$$

Substituting from Eq. (3.3) into the **first term** on the right of Eq. (3.8) (neglecting terms as before) gives

$$f^{(0)} f_1^{(0)}\left(\Phi^{(1)^*} + \Phi_1^{(1)^*} - \Phi^{(1)} - \Phi_1^{(1)}\right), \tag{3.9}$$

since

$$f^{(0)^*} f_1^{(0)^*} = f^{(0)} f_1^{(0)}.$$

The **second term** on the right of Eq. (3.8) involves space-derivatives. Thus we may write $f^{(0)}$ in place of $f^{(1)}$and obtain

$$f^{(0)^*} f_1^{(0)^*}\,\nabla_x \log f_1^{(0)^*} + f_1^{(0)^*} f^{(0)^*}\,\nabla_x \log f^{(0)^*} = f^{(0)} f_1^{(0)}\,\nabla_x \log\left[f_1^{(0)^*} f^{(0)^*}\right]$$

and

$$\begin{aligned}
&\nabla_x \log\Big[f_1^{(0)^*} f^{(0)^*}\Big] \\
&\quad = \frac{2}{n}\,\nabla_x n - \frac{3}{T}\,\nabla_x T + \frac{m}{2kT^2}\,\nabla_x T\left(\|v_1^* - c_0\|^2 + \|v^* - c_0\|^2\right) \\
&\qquad + \frac{m}{kT}(\nabla_x c_0)\Big((v_1^* - c_0) + (v^* - c_0)\Big) \\
&\quad = \cdots + \frac{m}{2kT^2}\,\nabla_x T\left(\|v_1 - c_0\|^2 + \|v - c_0\|^2\right) \\
&\qquad + \frac{m}{kT}(\nabla_x c_0)\Big((v_1 - c_0) + (v - c_0)\Big).
\end{aligned}$$

The integral on the right-hand side of Eq. (3.1) gives

$$\begin{aligned}
I &= \int\!\!\int \sigma e\cdot\Big(f^{(0)} f_1^{(0)}\,\nabla_x \log\Big[f_1^{(0)^*} f^{(0)^*}\Big]\Big)\sigma^2 (v_1 - v)\cdot e\,de\,dv_1 \\
&= \frac{2}{n}\sigma^3 f^{(0)}\int f_1^{(0)}\int e\cdot\nabla_x n\,(v_1 - v)\cdot e\,de\,dv_1 \\
&\quad - \frac{3}{T}\sigma^3 f^{(0)}\int f_1^{(0)}\int e\cdot\nabla_x T\,(v_1 - v)\cdot e\,de\,dv_1 \\
&\quad + \frac{m}{2kT^2}\sigma^3 f^{(0)}\int f_1^{(0)}\int e\cdot\nabla_x T\left(\|v_1 - c_0\|^2 + \|v - c_0\|^2\right)(v_1 - v)\cdot e\,de\,dv_1 \\
&\quad + \frac{m}{kT}\sigma^3 f^{(0)}\int f_1^{(0)}\int e\cdot(\nabla_x c_0)\Big((v_1 - c_0) + (v - c_0)\Big)(v_1 - v)\cdot e\,de\,dv_1.
\end{aligned} \tag{3.10}$$

According to Ref. [7, Formula 16.8,2] we have

$$\int e\,(v_1 - v)\cdot e\,de = \frac{2\pi}{3}\,(v_1 - v).$$

Thus, Eq. (3.10) implies

$$\begin{aligned}
I &= \frac{2\pi}{3}\,\frac{2}{n}\,\sigma^3 f^{(0)}\int f_1^{(0)}(v_1 - v)\cdot\nabla_x n\,dv_1 \\
&\quad - \frac{2\pi}{3}\,\frac{3}{T}\,\sigma^3 f^{(0)}\int f_1^{(0)}(v_1 - v)\cdot\nabla_x T\,dv_1 \\
&\quad + \frac{2\pi}{3}\,\frac{m}{2kT^2}\,\sigma^3 f^{(0)}\int f_1^{(0)}(v_1 - v)\cdot\nabla_x T\left(\|v_1 - c_0\|^2 + \|v - c_0\|^2\right)dv_1 \\
&\quad + \frac{2\pi}{3}\,\frac{m}{kT}\,\sigma^3 f^{(0)}\int f_1^{(0)}(v_1 - v)\cdot(\nabla_x c_0)\Big((v_1 - c_0) + (v - c_0)\Big)dv_1.
\end{aligned} \tag{3.11}$$

Note that (cf. Eq. (3.2))

$$\int f_1^{(0)}(v_1 - c_0) \cdot \nabla_x T \left(\|v_1 - c_0\|^2 + \|v - c_0\|^2\right) dv_1 = 0,$$

$$\int f_1^{(0)}(v - c_0) \cdot \nabla_x T \left(\|v_1 - c_0\|^2 + \|v - c_0\|^2\right) dv_1$$
$$= (v - c_0) \cdot \nabla_x T n \left[\frac{3kT}{m} + \|v - c_0\|^2\right],$$

(cf. Eq. (A.1))

$$\int f_1^{(0)}(v_1 - c_0) \cdot (\nabla_x c_0)\Big((v_1 - c_0) + (v - c_0)\Big) dv_1$$
$$= \int f_1^{(0)}(v_1 - c_0) \cdot (\nabla_x c_0)(v_1 - c_0)\, dv_1 = n\, \frac{kT}{m}\, \mathrm{div}(c_0)$$

and

$$\int f_1^{(0)}(v - c_0) \cdot (\nabla_x c_0)\Big((v_1 - c_0) + (v - c_0)\Big) dv_1$$
$$= n(v - c_0) \cdot (\nabla_x c_0)(v - c_0).$$

Thus, Eq. (3.11) implies

$$\begin{aligned} I = {} & -\frac{2\pi}{3}\, \frac{2}{n}\, \sigma^3 f^{(0)}\, n(v - c_0) \cdot \nabla_x n + \frac{2\pi}{3}\, \frac{3}{T}\, \sigma^3 f^{(0)}\, n(v - c_0) \cdot \nabla_x T \\ & - \frac{2\pi}{3}\, \frac{m}{2kT^2}\, \sigma^3 f^{(0)}(v - c_0) \cdot \nabla_x T\, n\left[\frac{3kT}{m} + \|v - c_0\|^2\right] \\ & + \frac{2\pi}{3}\, \frac{m}{kT}\, \sigma^3 f^{(0)}\left[n\, \frac{kT}{m}\, \mathrm{div}(c_0) - n(v - c_0) \cdot (\nabla_x c_0)(v - c_0)\right] \\ = {} & -\frac{2\pi}{3}\, n\sigma^3 f^{(0)}\, \frac{2}{n}\, (v - c_0) \cdot \nabla_x n \\ & - \frac{2\pi}{3}\, n\sigma^3 f^{(0)}(v - c_0) \cdot \nabla_x T\left[-\frac{3}{2T} + \frac{m}{2kT^2}\, \|v - c_0\|^2\right] \\ & + \frac{2\pi}{3}\, n\sigma^3 f^{(0)}\left[\mathrm{div}(c_0) - \frac{m}{kT}(v - c_0) \cdot (\nabla_x c_0)(v - c_0)\right]. \end{aligned}$$

When multiplying with $\psi = 1,\ v - c_0,\ \|v - c_0\|^2$and integrating with respect to v, many terms vanish. One obtains (cf. Eq. (A.1))

$$\int dv\, I = \frac{2\pi}{3}\, n\sigma^3\left[n\, \mathrm{div}(c_0) - \frac{m}{kT}\, \frac{kTn}{m}\, \mathrm{div}(c_0)\right] = 0, \tag{3.12}$$

(cf. Eqs. (A.2), (A.4), (A.3))

$$\begin{aligned}\int dv\,(v-c_0)\,I\\ &= -\frac{2\pi}{3}\,n\sigma^3\,\frac{2}{n}\,\frac{kTn}{m}\,\nabla_x n + \frac{2\pi}{3}\,n\sigma^3\,\frac{3}{2T}\,\frac{kTn}{m}\,\nabla_x T\\ &\quad -\frac{2\pi}{3}\,n\sigma^3\,\frac{m}{2kT^2}\,5n\left(\frac{kT}{m}\right)^2\nabla_x T\\ &= -\frac{2\pi}{3}\,n\sigma^3\,\frac{2kT}{m}\,\nabla_x n + \frac{2\pi}{3}\,n\sigma^3\,\nabla_x T\left[\frac{3kn}{2\,m}-\frac{5kn}{2\,m}\right]\\ &= -\frac{2\pi}{3}\,n\sigma^3\,\frac{2kT}{m}\,\nabla_x n - \frac{2\pi}{3}\,n\sigma^3\,\frac{kn}{m}\,\nabla_x T = -\frac{2\pi}{3m}\,\sigma^3\,\nabla_x(kn^2T)\end{aligned} \tag{3.13}$$

and (cf. Eq. (A.6))

$$\begin{aligned}\int dv\,\|v-c_0\|^2\,I &= \frac{2\pi}{3}n\sigma^3\,\mathrm{div}(c_0)\,\frac{3kTn}{m} - \frac{2\pi}{3}n\sigma^3\,\frac{m}{kT}\,5n\left(\frac{kT}{m}\right)^2\mathrm{div}(c_0)\\ &= \frac{2\pi}{3}n\sigma^3\,\mathrm{div}(c_0)\left[\frac{3kTn}{m}-\frac{5kTn}{m}\right]\\ &= -\frac{2\pi}{3}n\sigma^3\,\mathrm{div}(c_0)\,\frac{2kTn}{m}.\end{aligned} \tag{3.14}$$

Note that the corresponding integrals of the term Eq. (3.9) are zero.

3.3. Comparison of Both Sides

From Eqs. (3.4), (3.12), one obtains

$$\frac{D}{Dt}\,n + n\,\mathrm{div}(c_0) = 0. \tag{3.15}$$

This equation is identical with Ref. [7, (16.33,3)].

From Eqs. (3.6), (3.13) one obtains

$$n\frac{D}{Dt}\,c_0 + \frac{1}{m}\,\nabla_x(k\,nT) + \frac{2\pi}{3m}\,\sigma^3\,\nabla_x(kn^2T) = 0,$$

or

$$n\frac{D}{Dt}\,c_0 + \frac{1}{m}\,\nabla_x\left[knT\left[1+\frac{2\pi}{3}\,\sigma^3\,n\right]\right] = 0. \tag{3.16}$$

Introducing (cf. Ref. [7, (16.33,2)])

$$p_0 = knT\Big[1 + \frac{2\pi}{3}\,\sigma^3\, n\Big], \tag{3.17}$$

and up to some notations, Eq. (3.16) is identical with Ref. [7, Formula 16.33,4]. This equation of state is in agreement with that obtained from the virial.[1]

From Eqs. (3.7), (3.14), one obtains

$$\frac{3kT}{m}\,\frac{D}{Dt}\,n + \frac{3kn}{m}\,\frac{D}{Dt}\,T + \frac{5nkT}{m}\,\mathrm{div}(c_0) + \frac{2\pi}{3}\,n\sigma^3\,\mathrm{div}(c_0)\,\frac{2kTn}{m} = 0$$

or, using Eq. (3.15),

$$\frac{3kn}{m}\,\frac{D}{Dt}\,T + kT\,\mathrm{div}(c_0)\,\frac{2n}{m}\Big[1 + \frac{2\pi}{3}\,n\sigma^3\Big] = 0,$$

i.e.,

$$\frac{D}{Dt}\,T + \frac{2}{3}\,T\,\mathrm{div}(c_0)\Big[1 + \frac{2\pi}{3}\,n\sigma^3\Big] = 0. \tag{3.18}$$

Taking into account Eq. (3.17), this equation is identical with Ref. [7, formula 16.33,5].

Equations (3.15), (3.16), (3.18) are the first order approximations to the equations of continuity, momentum, and energy. These are the Euler equations with the hydrostatic pressure given by Eq. (3.17) and they are identical to those obtained for the Enskog equation (recall that for simplicity χ was taken as unity). For future work, the Chapman-Enskog analysis may be continued to evaluate the transport coefficients (cf. Ref. [6, Ch. V.6]) by computing the collisional transfer of momentum, energy, and for CBA, mass. We anticipate that, as with the Enskog equation, the resulting viscosity, thermal conductivity, and self-diffusion coefficient will be in good agreement with the results already obtained by Green-Kubo analysis (cf. Ref. [1,15]).

APPENDIX: MOMENTS OF A GAUSSIAN VARIABLE

Let $\xi = v - c_0$. Then

$$\int dv f^{(0)}\,\xi\cdot A\,\xi = \int dv f^{(0)} \sum_{j,k} \xi_j\, a_{j,k}\, \xi_k = \frac{kTn}{m}\,[a_{1,1} + a_{2,2} + a_{3,3}], \tag{A.1}$$

$$\int dv f^{(0)} \xi_i \xi \cdot b = \int dv f^{(0)} \xi_i^2 b_i = \frac{kTn}{m} b_i, \tag{A.2}$$

$$\int dv f^{(0)} \xi_i \xi \cdot A \xi = \int dv f^{(0)} \xi_i \sum_{j,k} \xi_j a_{j,k} \xi_k = 0, \tag{A.3}$$

$$\int dv f^{(0)} \xi_i \xi \cdot b \|\xi\|^2 = \int dv f^{(0)} \xi_i^2 b_i \|\xi\|^2 = n b_i \left(\frac{kT}{m}\right)^2 [1+1+3], \tag{A.4}$$

$$\int dv f^{(0)} \|\xi\|^4 = \int dv f^{(0)} (\xi_1^2 + \xi_2^2 + \xi_3^2)^2 = 15n \left(\frac{kT}{m}\right)^2 \tag{A.5}$$

and

$$\begin{aligned}\int dv f^{(0)} \|\xi\|^2 \xi \cdot A \xi &= \int dv f^{(0)} \|\xi\|^2 \sum_{j,k} \xi_j a_{j,k} \xi_k = \int dv f^{(0)} \sum_i \xi_i^2 \sum_j \xi_j^2 a_{j,j} \\ &= n\left(\frac{kT}{m}\right)^2 [3a_{1,1} + a_{2,2} + a_{3,3} + a_{1,1} + 3a_{2,2} + a_{3,3} + a_{1,1} + a_{2,2} + 3a_{3,3}] \\ &= 5n\left(\frac{kT}{m}\right)^2 [a_{1,1} + a_{2,2} + a_{3,3}]. \end{aligned} \tag{A.6}$$

These formulas follow from elementary properties of one-dimensional Gaussian random variables, in particular, $E\eta^4 = 3(E\eta^2)^2$, i.e.,

$$\frac{1}{n}\int dv f^{(0)} \|\xi_i\|^4 = 3\left[\frac{1}{n}\int dv f^{(0)} \|\xi_i\|^2\right]^2 = 3\left(\frac{kT}{m}\right)^2.$$

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