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The Limiting Kinetic Equation of the Consistent Boltzmann Algorithm for Dense Gases

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This paper establishes a theoretical foundation for the Consistent Boltzmann Algorithm (CBA) by deriving the limiting kinetic equation. The formulation is similar to the proof by one of the authors that the Boltzmann equation is the limiting kinetic equation for Direct Simulation Monte Carlo [W. Wagner, *J. Statist. Phys.* **66**:1011 (1992)]. For a simplified model distilled from CBA, the limiting equation is solved numerically, and very good agreement with the predictions of the theory is found.

KEY WORDS: Kinetic theory; Enskog equation; direct simulation Monte Carlo; Boltzmann equation; consistent Boltzmann Algorithm; dense gases.

1. INTRODUCTION

Direct Simulation Monte Carlo (DSMC) is presently the most widely used numerical algorithm in kinetic theory.[3] The limiting kinetic equation for DSMC is the nonlinear Boltzmann equation[16] so its application is restricted to dilute gases. In DSMC, particle pairs are randomly chosen to collide according to the collision probability for the interparticle potential. For example, for the hard sphere potential this probability is proportional to the particles' relative speed. The post-collision velocities are determined by randomly selecting the collision angles and the number of collisions each time step is computed from the local collision frequency. Note that in DSMC particles can be chosen to collide even if their actual trajectories do *not* overlap.

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Recently, the Consistent Boltzmann Algorithm (CBA) was introduced as a simple variant of DSMC for dense gases.[1] Although CBA can be generalized to any equation of state[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 additions. First, when a pair collides the unit apse vector, e, that is, the unit vector parallel to the line connecting the centers at impact, is computed from the pre- and post-collision velocities of the particles. Each particle is displaced a distance σ, one in the direction e and the other in the direction $-e$ (see Fig. 1). Second, the dense hard sphere collision frequency, which contains the so-called Y-factor, is used. With these two simple additions CBA yields the hard sphere equation of state at all densities.

Frezzotti[6] and others[11] have proposed dense gas variants of DSMC based on the Enskog equation.[13] The main advantages of CBA over Enskog-based schemes are its simplicity in implementation and almost negligible effect on computational efficiency for a standard DSMC program. The transport coefficients for CBA, obtained by Green–Kubo analysis, are similar to those of the Enskog equation.[1] As already mentioned, CBA can be extended to potentials other than hard spheres. Besides the standard problems in kinetic theory, CBA has proved useful in the study of granular materials[8] and nuclear physics.[9]

Until now the principal deficiency of the Consistent Boltzmann Algorithm was that it lacked a complete theoretical foundation. This paper establishes much of that foundation by deriving the limiting kinetic equation for CBA. In the next section we give a description of the CBA by introducing the corresponding Markov process. In Section 3 we formally derive the equation satisfied by the limit of the empirical measures of this

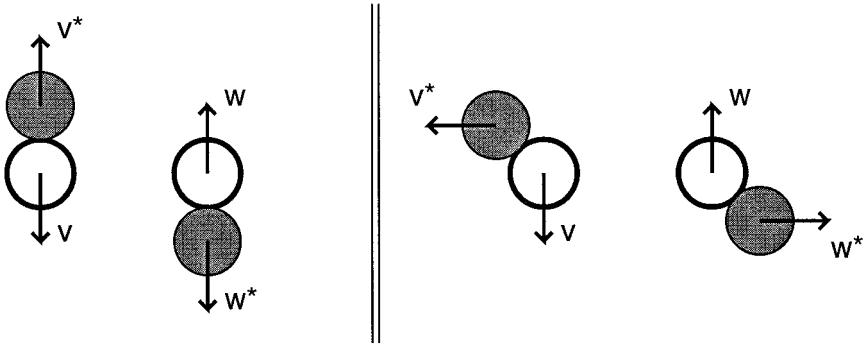

Fig. 1. Two illustrations of CBA collision displacement for different apse vectors. Before collision the particles have position and velocity (x, v), (y, w). After collision the velocities are v^* and w^*; the shifted positions are indicated by shaded particles.

process when the number of particles tends to infinity. In Section 4 we transform the limiting equation for measure-valued functions into a form for densities. The relationship between this equation and other kinetic equations, including the Enskog equation, is outlined in Section 5. Various sources of numerical error in the CBA and their influence on the limiting equation are discussed in Section 6. In order to illustrate the general results, we consider a simplified model in Section 7. For this toy model, the stochastic process and the limiting equation are solved numerically, and very good agreement with the predictions of the theory is found. The paper closes with some concluding remarks in Section 8.

2. THE MARKOV PROCESS RELATED TO THE CBA

The interaction of two particles (x, v) and (y, w) is determined by the functions

$$x^*(x, v, y, w, e), \qquad y^*(x, v, y, w, e), \qquad v^*(x, v, y, w, e),$$
$$w^*(x, v, y, w, e), \qquad e \in \mathscr{S}^2$$

describing the post-collision positions and the post-collision velocities, respectively. These functions are defined as

$$v^*(x, v, y, w, e) = v + e(e, w - v), \qquad w^*(x, v, y, w, e) = w - e(e, w - v) \tag{2.1}$$

and

$$\begin{aligned} x^*(x, v, y, w, e) &= x + \sigma \frac{(v^* - w^*) - (v - w)}{\|(v^* - w^*) - (v - w)\|} \\ y^*(x, v, y, w, e) &= y - \sigma \frac{(v^* - w^*) - (v - w)}{\|(v^* - w^*) - (v - w)\|} \end{aligned} \tag{2.2}$$

where $x, y \in \mathscr{R}^3$, $v, w \in \mathscr{R}^3$, $\mathscr{S}^2 \subset \mathscr{R}^3$ is the unit sphere, and $(\cdot, \cdot)$, $\|\cdot\|$ denote the scalar product and the Euclidean norm in $\mathscr{R}^3$, respectively. If $(e, v - w) = 0$ then define $x^* = x$ and $y^* = y$. The parameter $\sigma \geqslant 0$ is interpreted as the diameter of the particles. The standard Boltzmann collision transformation is recovered in the case $\sigma = 0$.

Remark 2.1. We consider the position space $\mathscr{R}^3$ in order to avoid the discussion of boundary effects.

Using (2.1) one obtains

$$(v^* - w^*) - (v - w) = 2e(e, w - v) \tag{2.3}$$

and (2.2) takes the form

$$x^* = x + \sigma e \operatorname{sign}(e, w - v), \qquad y^* = y - \sigma e \operatorname{sign}(e, w - v) \tag{2.4}$$

or

$$x^* = x + \psi(v, w, e), \qquad y^* = y - \psi(v, w, e) \tag{2.5}$$

using the notation

$$\psi(v, w, e) = \sigma e \operatorname{sign}(e, w - v) \tag{2.6}$$

From (2.3) one obtains

$$(e, w^* - v^*) = (e, w - v) + 2(e, v - w) = -(e, w - v)$$

and

$$\psi(v^*, w^*, e) = -\psi(v, w, e) = \psi(w, v, e) \tag{2.7}$$

so that

$$(x^{**}, v^{**}, y^{**}, w^{**}) = (x, v, y, w) \tag{2.8}$$

The Markov process related to the collision step of the CBA has states of the form

$$z = ((x_1, v_1), \ldots, (x_n, v_n)) \in (\mathscr{R}^3 \times \mathscr{R}^3)^n$$

and the infinitesimal generator

$$\mathscr{A}(\Phi)(z) = \frac{1}{2n} \sum_{1 \leqslant i \neq j \leqslant n} \int_{\mathscr{S}^2} Q(z, i, j, e)[\Phi(J(z, i, j, e)) - \Phi(z)]\, de \tag{2.9}$$

where the jump transformation is

$$[J(z, i, j, e)]_k = \begin{cases} (x_k, v_k), & \text{if } k \neq i, j \\ (x^*, v^*), & \text{if } k = i \\ (y^*, w^*), & \text{if } k = j \end{cases} \tag{2.10}$$

and the functions x^*, v^*, y^*, w^* depend on the arguments x_i, v_i, x_j, v_j, e. The intensity function has the form

$$Q(z, i, j, e) = Y\left(\frac{1}{n}\sum_{k=1}^{n} g(x_i, x_k)\right) h(x_i, x_j)\, B(v_i, v_j, e) \tag{2.11}$$

The functions h and g are mollifying kernels (non-negative approximations of Dirac's delta-function), and will be specified when necessary. The function B is the Boltzmann collision kernel. In the case of hard spheres the collision kernel takes the form

$$B(v, w, e) = \text{const}\ |(e, w - v)| \tag{2.12}$$

Finally, the notation used here for the function Y follows that of the "Y-factor" from kinetic theory.[13] This function is continuous and strictly positive with $Y(\varrho)$ going to infinity as $\varrho \to \varrho_m$ where ϱ_m is the density at close-packing.

3. DERIVATION OF THE LIMITING EQUATION

The Markov process $Z(t) = (X_i(t), V_i(t))_{i=1}^n$ defined by the generator (2.9) satisfies

$$\Phi(Z(t)) = \Phi(Z(0)) + \int_0^t \mathscr{A}(\Phi)(Z(s))\, ds + M(t), \qquad t \geqslant 0 \tag{3.1}$$

where Φ is an appropriate test function, and $M(t)$ is some martingale term. We consider the function

$$\Phi(z) = \frac{1}{n}\sum_{i=1}^{n} \varphi(x_i, v_i) \tag{3.2}$$

so that

$$\Phi(Z(t)) = \frac{1}{n}\sum_{i=1}^{n} \varphi(X_i(t), V_i(t)) = \int_{\mathscr{R}^3 \times \mathscr{R}^3} \varphi(x, v)\, v^{(n)}(t, dx, dv)$$

where $v^{(n)}$ are the empirical measures of the particle process. According to (2.9)–(2.11), one obtains

$$\begin{aligned}\mathscr{A}(\Phi)(z) = \frac{1}{2n^2} \sum_{1 \leqslant i \neq j \leqslant n} \int_{\mathscr{S}^2} & Y\left(\frac{1}{n}\sum_{k=1}^{n} g(x_i, x_k)\right) h(x_i, x_j)\, B(v_i, v_j, e) \\ & \times [\varphi(x^*, v^*) - \varphi(x_i, v_i) + \varphi(y^*, w^*) - \varphi(x_j, v_j)]\, de\end{aligned}$$

and

$$\begin{aligned}\mathscr{A}(\Phi)(Z(s)) = \tfrac{1}{2}\int_{\mathscr{R}^3\times\mathscr{R}^3}\int_{\mathscr{R}^3\times\mathscr{R}^3}\int_{\mathscr{S}^2} Y\left(\int_{\mathscr{R}^3} g(x,u)\, v^{(n)}(s, du, \mathscr{R}^3)\right)\\ \times h(x, y)\, B(v, w, e)\\ \times [\varphi(x^*, v^*) - \varphi(x, v) + \varphi(y^*, w^*) - \varphi(y, w)]\, de\\ \times v^{(n)}(s, dx, dv)\, v^{(n)}(s, dy, dw) + O(n^{-1})\end{aligned}$$

where the functions x^*, v^*, y^*, w^* depend on the arguments x, v, y, w, e.

Suppose that the following relations are fulfilled as $n \to \infty$,

$$v^{(n)}(t) \to P(t), \qquad M^{(n)}(t) \to 0, \qquad \forall t \geqslant 0 \tag{3.3}$$

for some deterministic measure-valued function $P(t)$. Under certain assumptions concerning this convergence, one can conclude from (3.1) that the limit $P(t)$ satisfies the equation

$$\begin{aligned}&\int_{\mathscr{R}^3\times\mathscr{R}^3} \varphi(x, v)\, P(t, dx, dv)\\ &= \int_{\mathscr{R}^3\times\mathscr{R}^3} \varphi(x, v)\, P_0(dx, dv)\\ &\quad + \int_0^t \tfrac{1}{2}\int_{\mathscr{R}^3\times\mathscr{R}^3}\int_{\mathscr{R}^3\times\mathscr{R}^3}\int_{\mathscr{S}^2} Y\left(\int_{\mathscr{R}^3} g(x,u)\, P(s, du, \mathscr{R}^3)\right) h(x, y)\, B(v, w, e)\\ &\quad \times [\varphi(x^*, v^*) - \varphi(x, v) + \varphi(y^*, w^*) - \varphi(y, w)]\, de\\ &\quad \times P(s, dx, dv)\, P(s, dy, dw)\, ds\end{aligned}$$

The differential form with respect to t is

$$\begin{aligned}&\frac{d}{dt}\int_{\mathscr{R}^3\times\mathscr{R}^3} \varphi(x, v)\, P(t, dx, dv)\\ &= \frac{1}{2}\int_{\mathscr{R}^3\times\mathscr{R}^3}\int_{\mathscr{R}^3\times\mathscr{R}^3}\int_{\mathscr{S}^2} Y\left(\int_{\mathscr{R}^3} g(x,u)\, P(t, du, \mathscr{R}^3)\right) h(x, y)\, B(v, w, e)\\ &\quad \times [\varphi(x^*, v^*) - \varphi(x, v) + \varphi(y^*, w^*) - \varphi(y, w)]\, de\\ &\quad \times P(t, dx, dv)\, P(t, dy, dw)\end{aligned} \tag{3.4}$$

with the initial condition

$$P_0 = \lim_{n\to\infty} v^{(n)}(0) \tag{3.5}$$

In the case of non-splitting (free flow included) a term of the form

$$\sum_{i=1}^{n} (v_i, \nabla_{x_i}) \tag{3.6}$$

is added to the generator, where ∇ denotes the gradient. Applied to the function (3.2), the operator (3.6) gives

$$\frac{1}{n} \sum_{i=1}^{n} (v_i, (\nabla_x \varphi)(x_i, v_i))$$

so that additionally the term

$$\int_{\mathscr{R}^3 \times \mathscr{R}^3} (v, (\nabla_x \varphi)(x, v))\, P(t, dx, dv) \tag{3.7}$$

occurs at the right-hand side of Eq. (3.4).

The weak form (3.4) of the equation is convenient for obtaining conservation properties (put $\varphi = 1,\ v,\ \|v\|^2$).

The crucial point in making the above derivation rigorous is to establish property (3.3). For the case of standard DSMC ($Y \equiv 1,\ \sigma = 0$), this was done in ref. 16. General results for stochastic systems with Boltzmann-type interaction were obtained in ref. 12. Some results covering Vlasov-type terms (like the Y-factor) can be found in ref. 7. We refer to ref. 17 concerning historical comments and an extended reference list.

4. TRANSFORMATION OF THE LIMITING EQUATION

Assume the measures have densities

$$P(t, dx, dv) = p(t, x, v)\, dx\, dv$$

and denote

$$\beta(x) = Y\left(\int_{\mathscr{R}^3} g(x, u)\, \varrho(t, u)\, du \right) \tag{4.1}$$

where

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

Assume that h is symmetric and

$$B(v, w, e) = B(v^*, w^*, e) = B(w, v, e) = B(v, w, -e) \tag{4.2}$$

Note that the kernel (2.12) satisfies (4.2).

Consider the right-hand side of Eq. (3.4). Applying the substitution $(v^*, w^*) \to (v, w)$, a substitution of variables in the position space, and properties (4.2), (2.7), (2.8), these terms take the form (cf. (2.5), (2.6))

$$\begin{aligned}
I_1 &= \tfrac{1}{2} \int_{\mathscr{R}^3} dx \int_{\mathscr{R}^3} dy \int_{\mathscr{R}^3} dv \int_{\mathscr{R}^3} dw \int_{\mathscr{S}^2} de \\
&\quad \times \beta(x)\, h(x, y)\, B(v, w, e)\, \varphi(x + \psi(v, w, e), v^*)\, p(t, x, v)\, p(t, y, w) \\
&= \tfrac{1}{2} \int_{\mathscr{R}^3} dx \int_{\mathscr{R}^3} dy \int_{\mathscr{R}^3} dv \int_{\mathscr{R}^3} dw \int_{\mathscr{S}^2} de \\
&\quad \times \beta(x)\, h(x, y)\, B(v^*, w^*, e)\, \varphi(x + \psi(v^*, w^*, e), v)\, p(t, x, v^*)\, p(t, y, w^*) \\
&= \tfrac{1}{2} \int_{\mathscr{R}^3} dx \int_{\mathscr{R}^3} dy \int_{\mathscr{R}^3} dv \int_{\mathscr{R}^3} dw \int_{\mathscr{S}^2} de \\
&\quad \times \beta(x)\, h(x, y)\, B(v, w, e)\, \varphi(x + \psi(w, v, e), v)\, p(t, x, v^*)\, p(t, y, w^*) \\
&= \tfrac{1}{2} \int_{\mathscr{R}^3} dx \int_{\mathscr{R}^3} dy \int_{\mathscr{R}^3} dv \int_{\mathscr{R}^3} dw \int_{\mathscr{S}^2} de\, B(v, w, e) \\
&\quad \times \beta(x + \psi(v, w, e))\, h(x + \psi(v, w, e), y)\, \varphi(x, v) \\
&\quad \times p(t, x, +\psi(v, w, e), v^*)\, p(t, y, w^*)
\end{aligned}$$

and

$$\begin{aligned}
I_2 &= \tfrac{1}{2} \int_{\mathscr{R}^3} dx \int_{\mathscr{R}^3} dy \int_{\mathscr{R}^3} dv \int_{\mathscr{R}^3} dw \int_{\mathscr{S}^2} de \\
&\quad \times \beta(x)\, h(x, y)\, B(v, w, e)\, \varphi(y + \psi(w, v, e), w^*)\, p(t, x, v)\, p(t, y, w) \\
&= \tfrac{1}{2} \int_{\mathscr{R}^3} dx \int_{\mathscr{R}^3} dy \int_{\mathscr{R}^3} dv \int_{\mathscr{R}^3} dw \int_{\mathscr{S}^2} de \\
&\quad \times \beta(x)\, h(x, y)\, B(v^*, w^*, e)\, \varphi(y + \psi(w^*, v^*, e), w)\, p(t, x, v^*)\, p(t, y, w^*) \\
&= \tfrac{1}{2} \int_{\mathscr{R}^3} dx \int_{\mathscr{R}^3} dy \int_{\mathscr{R}^3} dv \int_{\mathscr{R}^3} dw \int_{\mathscr{S}^2} de \\
&\quad \times \beta(x)\, h(x, y)\, B(v, w, e)\, \varphi(y + \psi(v, w, e), w)\, p(t, x, v^*)\, p(t, y, w^*)
\end{aligned}$$

$$= \tfrac{1}{2} \int_{\mathscr{R}^3} dx \int_{\mathscr{R}^3} dy \int_{\mathscr{R}^3} dv \int_{\mathscr{R}^3} dw \int_{\mathscr{S}^2} de$$

$$\times \beta(x)\, h(x,\, y + \psi(w, v, e))\, B(v, w, e)\, \varphi(y, w)\, p(t, x, v^*)$$

$$\times p(t,\, y + \psi(w, v, e), w^*)$$

$$= \tfrac{1}{2} \int_{\mathscr{R}^3} dx \int_{\mathscr{R}^3} dy \int_{\mathscr{R}^3} dv \int_{\mathscr{R}^3} dw \int_{\mathscr{S}^2} de$$

$$\times \beta(y)\, h(y,\, x + \psi(v, w, e))\, B(v, w, e)\, \varphi(x, v)\, p(t,\, y,\, w^*)$$

$$\times p(t,\, x + \psi(v, w, e), v^*)$$

Removing the test functions, one obtains

$$\frac{\partial}{\partial t} p(t, x, v) = \int_{\mathscr{R}^3} dy \int_{\mathscr{R}^3} dw \int_{\mathscr{S}^2} de\, B(v, w, e)$$

$$\times \left[\frac{\beta(x^*) + \beta(y)}{2} h(y, x^*)\, p(t, x^*, v^*)\, p(t,\, y,\, w^*) \right.$$

$$\left. - \frac{\beta(x) + \beta(y)}{2} h(x,\, y)\, p(t, x, v)\, p(t,\, y,\, w) \right] \tag{4.3}$$

Finally, taking into account the free flow term (3.7), we obtain the equation

$$\frac{\partial}{\partial t} p(t, x, v) + (v, \nabla_x)\, p(t, x, v)$$

$$= \int_{\mathscr{R}^3} dy \int_{\mathscr{R}^3} dw \int_{\mathscr{S}^2} de\, B(v, w, e)$$

$$\times \left[\frac{\beta(x^*) + \beta(y)}{2} h(y, x^*)\, p(t, x^*, v^*)\, p(t,\, y,\, w^*) \right.$$

$$\left. - \frac{\beta(x) + \beta(y)}{2} h(x,\, y)\, p(t, x, v)\, p(t,\, y,\, w) \right] \tag{4.4}$$

If

$$h(x,\, y) = h^{(n)}(x,\, y) \to \delta(x - y) \qquad (n \to \infty) \tag{4.5}$$

then Eq. (4.4) takes the form

$$\frac{\partial}{\partial t} p(t, x, v) + (v, \nabla_x)\, p(t, x, v)$$

$$= \int_{\mathscr{R}^3} dw \int_{\mathscr{S}^2} de\, B(v, w, e)[\beta(x^*)\, p(t, x^*, v^*)\, p(t, x^*, w^*)$$

$$- \beta(x)\, p(t, x, v)\, p(t, x, w)] \tag{4.6}$$

According to (4.1), if

$$g(x, y) = g^{(n)}(x, y) \to \delta(x - y) \qquad (n \to \infty) \tag{4.7}$$

then $\beta(x) = Y(\varrho(t, x))$, and Eq. (4.6) takes the form

$$\frac{\partial}{\partial t} p(t, x, v) + (v, \nabla_x)\, p(t, x, v)$$

$$= \int_{\mathscr{R}^3} dw \int_{\mathscr{S}^2} de\, B(v, w, e)[\, Y(\varrho(t, x^*))\, p(t, x^*, v^*)\, p(t, x^*, w^*)$$

$$- Y(\varrho(t, x))\, p(t, x, v)\, p(t, x, w)] \tag{4.8}$$

This is the *kinetic equation*, which is numerically solved by the CBA.

The rigorous derivation of the limiting equation from the stochastic particle system becomes much more difficult in the case (4.5), (4.7). Such a procedure for a one-dimensional model with strictly local interaction was carried out in ref. 4. Results for a discrete velocity Boltzmann equation were obtained in ref. 14. The Boltzmann case with small initial data was treated in ref. 10.

5. RELATED EQUATIONS

First we note that in the case $Y \equiv 1$, $\sigma = 0$ (cf. (2.2)) the *Boltzmann equation*

$$\frac{\partial}{\partial t} p(t, x, v) + (v, \nabla_x)\, p(t, x, v)$$

$$= \int_{\mathscr{R}^3} dw \int_{\mathscr{S}^2} de\, B(v, w, e)[\, p(t, x, v^*)\, p(t, x, w^*) - p(t, x, v)\, p(t, x, w)]$$

is derived from Eq. (4.8).

With

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

we obtain (cf. (2.4), (4.1), (4.7), (4.2))

$$\begin{aligned}
&\int_{\mathscr{S}^2} de\, B(v, w, e)\, \beta(x^*)\, p(t, x^*, v^*)\, p(t, x^*, w^*) \\
&\quad = \int_{\mathscr{S}^2_+} de\, B(v, w, e)\, \beta(x+\sigma e)\, p(t, x+\sigma e, v^*)\, p(t, x+\sigma e, w^*) \\
&\qquad + \int_{\mathscr{S}^2_-} de\, B(v, w, e)\, \beta(x-\sigma e)\, p(t, x-\sigma e, v^*)\, p(t, x-\sigma e, w^*) \\
&\quad = 2\int_{\mathscr{S}^2_-} de\, B(v, w, e)\, \beta(x-\sigma e)\, p(t, x-\sigma e, v^*)\, p(t, x-\sigma e, w^*) \\
&\quad = 2\int_{\mathscr{S}^2_+} de\, B(v, w, e)\, \beta(x+\sigma e)\, p(t, x+\sigma e, v^*)\, p(t, x+\sigma e, w^*)
\end{aligned}$$

so that Eq. (4.8) takes the form

$$\begin{aligned}
&\frac{\partial}{\partial t} p(t, x, v) + (v, \nabla_x)\, p(t, x, v) \\
&\quad = 2\int_{\mathscr{R}^3} dw \int_{\mathscr{S}^2_+} de\, B(v, w, e) \\
&\qquad \times [\, Y(\varrho(t, x+\sigma e))\, p(t, x+\sigma e, v^*)\, p(t, x+\sigma e, w^*) \\
&\qquad - Y(\varrho(t, x))\, p(t, x, v)\, p(t, x, w)\,]
\end{aligned} \tag{5.1}$$

Compare this equation with the *Enskog equation* (cf. [5, Ch. 16])

$$\begin{aligned}
&\frac{\partial}{\partial t} p(t, x, v) + (v, \nabla_x)\, p(t, x, v) \\
&\quad = 2\int_{\mathscr{R}^3} dw \int_{\mathscr{S}^2_+} de\, B(v, w, e) \\
&\qquad \times [\, Y(\varrho(t, x+\tfrac{1}{2}\sigma e))\, p(t, x, v^*)\, p(t, x+\sigma e, w^*) \\
&\qquad - Y(\varrho(t, x-\tfrac{1}{2}\sigma e))\, p(t, x, v)\, p(t, x-\sigma e, w)\,]
\end{aligned} \tag{5.2}$$

The *revised Enskog equation*[15] is the same as (5.2) with the Y-factor replaced with the local-equilibrium pair distribution function; a similar revision of CBA has not been investigated.

6. SOURCES OF ERROR IN THE CBA

Equation (4.8) has been derived in the limit $n \to \infty$ assuming that all other sources of error vanish. As in the Boltzmann case ($Y \equiv 1$, $\sigma = 0$) there are other forms of the limiting equation, in which the influence of different numerical errors can be seen.

The splitting of the free flow and the collision step leads to a *Δt-error*. This is reflected in a corresponding splitting of the limiting equation into (4.3) and

$$\frac{\partial}{\partial t} p(t, x, v) + (v, \nabla_x)\, p(t, x, v) = 0$$

During the collision simulation step a partition $\mathscr{R}^3 = C_1 \cup C_2 \cup \cdots$ of the position space into disjoint cells is used. This leads to a *Δx-error* and is reflected by the presence of the mollifying kernel

$$h(x, y) = \sum_l \frac{1}{|C_l|} \chi_{C_l}(x)\, \chi_{C_l}(y) \tag{6.1}$$

in the limiting equation (4.3). Here $|C_l|$ denotes the Lebesgue measure of the cell C_l, and χ is the indicator function.

Moreover, unlike the Boltzmann case, the jump processes in different cells are not independent from each other since particle positions change during collisions. This is inconvenient from a numerical point of view. Therefore the particles are sorted into cells only at the beginning of the collision time step and these subsystems evolve independently. While in the original process only particles in the same cell interact, in the approximate processes particles in different cells may interact if they were in the same cell at the beginning of the time step. Conversely, particles that begin the time step in different cells cannot interact even if a collision displaces them to the same cell during the time step.

This approximation leads to an *additional Δt-error*, which is reflected in the limiting equation in the following way. For each l, the initial state of the approximate process consists of all particles belonging to cell C_l. Its

evolution is determined by the generator (2.9)–(2.11), where the function h is replaced by

$$h_l(x, y) = \frac{1}{|C_l|} \tag{6.2}$$

and the sum is taken over the appropriately reduced set of indices. The corresponding limiting equation is (cf. (4.3))

$$\begin{aligned}\frac{\partial}{\partial s}\tilde{p}_l(s, x, v) = \frac{1}{|C_l|}\int_{\mathscr{R}^3} dy \int_{\mathscr{R}^3} dw \int_{\mathscr{S}^2} de\, B(v, w, e) \\ \times\left[\frac{\beta(x^*)+\beta(y)}{2}\tilde{p}_l(s, x^*, v^*)\,\tilde{p}_l(s, y, w^*)\right. \\ \left. -\frac{\beta(x)+\beta(y)}{2}\tilde{p}_l(s, x, v)\,\tilde{p}_l(s, y, w)\right], \qquad s \geqslant t\end{aligned} \tag{6.3}$$

with initial condition (cf. (3.5))

$$\tilde{p}_l(t, x, v) = \chi_{C_l}(x)\, p(t, x, v) \tag{6.4}$$

These equations are solved on the time interval $[t, t+\Delta t]$. Then the solution at the end of the time step is constructed as

$$p(t+\Delta t, x, v) = \sum_l \tilde{p}_l(t+\Delta t, x, v) \tag{6.5}$$

The time step in the simulations is selected such that only a small fraction of particles collide at each step so typically this error is small.

7. A TOY MODEL

As an illustrative example, in this section we consider an extremely simplified random walk model that is directly related to the Consistent Boltzmann Algorithm. Following the ideas from the previous sections, we derive a limiting kinetic equation, which may be expressed as a partial differential equation. This equation is solved numerically, illustrating the convergence behaviour of the stochastic system.

Consider a system where the particles do not have velocities but change their positions during an interaction. The evolution of the system is determined by the generator

$$\mathscr{A}(\Phi)(x) = \frac{B}{2n}\sum_{1 \leqslant i \neq j \leqslant n}\int_{\mathscr{S}^2} h(x_i, x_j)[\Phi(J(x, i, j, e)) - \Phi(x)]\, de \tag{7.1}$$

where $x=(x_1,...,x_n)\in(\mathscr{R}^3)^n$ and

$$[J(x,i,j,e)]_k=\begin{cases}x_k, & \text{if} \quad k\neq i,\ j\\ x_i+\sigma e, & \text{if} \quad k=i\\ x_j-\sigma e, & \text{if} \quad k=j\end{cases} \tag{7.2}$$

Compared with (2.9)–(2.11), the function B is a constant, since particle velocities are absent. For simplicity we take $Y=1$.

For $\Phi(x)=(1/n)\sum_{i=1}^n\varphi(x_i)$, one obtains

$$\mathscr{A}(\Phi)(x)=\frac{B}{2n^2}\sum_{1\leqslant i\neq j\leqslant n}\int_{\mathscr{S}^2}h(x_i,x_j)\times[\varphi(x_i+\sigma e)-\varphi(x_i)+\varphi(x_j-\sigma e)-\varphi(x_j)]\,de$$

and

$$\mathscr{A}(\Phi)(X(s))=\frac{B}{2}\int_{\mathscr{R}^3}\int_{\mathscr{R}^3}\int_{\mathscr{S}^2}h(x,y)[\varphi(x+\sigma e)-\varphi(x)+\varphi(y-\sigma e)-\varphi(y)]\times de\,v^{(n)}(s,dx)\,v^{(n)}(s,dy)+O(n^{-1})$$

so that

$$\frac{d}{dt}\int_{\mathscr{R}^3}\varphi(x)\,P(t,dx)=\frac{B}{2}\int_{\mathscr{R}^3}\int_{\mathscr{R}^3}\int_{\mathscr{S}^2}h(x,y)[\varphi(x+\sigma e)-\varphi(x)+\varphi(y-\sigma e)-\varphi(y)]\times de\,P(t,dx)\,P(t,dy) \tag{7.3}$$

in analogy with (3.4).

First we suppose that the limiting measures $P(t,dx)$ have densities $p(t,x)$. From

$$I=\int_{\mathscr{R}^3}dx\int_{\mathscr{R}^3}dy\int_{\mathscr{S}^2}de\,h(x,y)\,\varphi(x+\sigma e)\,p(t,x)\,p(t,y)$$

$$=\int_{\mathscr{R}^3}dx\int_{\mathscr{R}^3}dy\int_{\mathscr{S}^2}de\,h(x-\sigma e,y)\,\varphi(x)\,p(t,x-\sigma e)\,p(t,y)$$

and

$$\int_{\mathscr{R}^3} dx \int_{\mathscr{R}^3} dy \int_{\mathscr{S}^2} de\, h(x, y)\, \varphi(y - \sigma e)\, p(t, x)\, p(t, y)$$

$$= \int_{\mathscr{R}^3} dx \int_{\mathscr{R}^3} dy \int_{\mathscr{S}^2} de\, h(x, y + \sigma e)\, \varphi(y)\, p(t, x)\, p(t, y + \sigma e)$$

$$= \int_{\mathscr{R}^3} dx \int_{\mathscr{R}^3} dy \int_{\mathscr{S}^2} de\, h(y, x + \sigma e)\, \varphi(x)\, p(t, y)\, p(t, x + \sigma e) = I$$

one obtains

$$\frac{\partial}{\partial t} p(t, x) = B \int_{\mathscr{R}^3} dy \int_{\mathscr{S}^2} de \times [h(y, x + \sigma e)\, p(t, x + \sigma e)\, p(t, y) - h(x, y)\, p(t, x)\, p(t, y)] \tag{7.4}$$

or, with (4.5),

$$\frac{\partial}{\partial t} p(t, x) = B \int_{\mathscr{S}^2} [p(t, x + \sigma e)^2 - p(t, x)^2]\, de \tag{7.5}$$

This *basic equation* for the toy model is the analogue of the kinetic equation (4.8).

Equation (6.3) takes the form

$$\frac{\partial}{\partial s} \tilde{p}_l(s, x) = \frac{B}{|C_l|} \int_{\mathscr{R}^3} dy \int_{\mathscr{S}^2} de[\tilde{p}_l(s, x + \sigma e)\, \tilde{p}_l(s, y) - \tilde{p}_l(s, x)\, \tilde{p}_l(s, y)]$$

$$= \frac{B}{|C_l|} \int_{\mathscr{R}^3} \tilde{p}_l(s, y)\, dy \int_{\mathscr{S}^2} [\tilde{p}_l(s, x + \sigma e) - \tilde{p}_l(s, x)]\, de, \qquad s \geqslant t \tag{7.6}$$

Note that (7.3) implies

$$\frac{d}{dt} \int_{\mathscr{R}^3} \varphi(x)\, P(t, dx) = 0$$

for $\varphi(x) = 1$ (mass conservation) and $\varphi(x) = x$ (conservation of the mean), and any symmetric h. Using mass conservation we obtain

$$\int_{\mathscr{R}^3} \tilde{p}_l(s, y)\, dy = \int_{\mathscr{R}^3} \tilde{p}_l(t, y)\, dy = \int_{C_l} p(t, y)\, dy, \qquad s \geqslant t$$

which is used to simplify (7.6). Finally, the approximate equations (6.3)–(6.5) take the form

$$\frac{\partial}{\partial s}\tilde{p}_l(s, x) = \frac{B}{|C_l|}\int_{C_l} p(t, y)\, dy \int_{\mathscr{S}^2} [\tilde{p}_l(s, x+\sigma e) - \tilde{p}_l(s, x)]\, de, \qquad s \geqslant t \tag{7.7}$$

$$\tilde{p}_l(t, x) = \chi_{C_l}(x)\, p(t, x) \tag{7.8}$$

$$p(t+\Delta t, x) = \sum_l \tilde{p}_l(t+\Delta t, x) \tag{7.9}$$

Note that Eqs. (7.7) are linear. Compared with (7.5), one factor of the quadratic terms has been replaced by a function constant in space and time.

In the *one-dimensional case* we choose

$$B = \frac{D}{\sigma^2} \tag{7.10}$$

for some constant $D > 0$, so that Eq. (7.5) takes the form

$$\frac{\partial}{\partial t} p(t, x) = D\,\frac{p(t, x+\sigma)^2 + p(t, x-\sigma)^2 - 2p(t, x)^2}{\sigma^2} \tag{7.11}$$

giving in the limit $\sigma \to 0$ the partial differential equation

$$\frac{\partial}{\partial t} p(t, x) = D\,\frac{\partial^2}{\partial x^2} p(t, x)^2 \tag{7.12}$$

Note that the unit sphere degenerates to the set $\{-1; 1\}$, where each point is given unit weight. An alternative way of writing (7.12) is

$$\frac{\partial}{\partial t} p(t, x) = \frac{\partial}{\partial x}\,\mathscr{D}\,\frac{\partial}{\partial x} p(t, x)$$

where $\mathscr{D} = 2Dp(x, t)$ can be viewed as a nonlinear diffusion coefficient.

Next we consider a situation where the limiting measures $P(t, dx)$ are not absolutely continuous with respect to Lebesgue measure. Starting on the *grid*

$$G = \{i\sigma : i = ..., -1, 0, 1, ...\}$$

the process remains there, so that the limiting measures are concentrated on G. Using the notations

$$x = i\sigma, \qquad y = j\sigma, \qquad p(t, x) = P(t, \{x\})$$

and considering the test functions $\varphi_i(y) = \chi_{\{x\}}(y) = \delta_{i,j}$, one obtains from (7.3)

$$\frac{d}{dt} p(t, x) = B \sum_j \int_{\mathscr{S}^0} [h(y, x+\sigma e)\, p(t, x+\sigma e)\, p(t, y) - h(x, y)\, p(t, x)\, p(t, y)]\, de \tag{7.13}$$

in analogy with (7.4). Choosing

$$h(x, y) = \sum_l \chi_{\{l\sigma\}}(x)\, \chi_{\{l\sigma\}}(y) = \delta_{i,j} \tag{7.14}$$

and assuming (7.10), Eq. (7.13) takes the form

$$\frac{d}{dt} p(t, x) = D \frac{p(t, x+\sigma)^2 + p(t, x-\sigma)^2 - 2p(t, x)^2}{\sigma^2}, \qquad x \in G \tag{7.15}$$

in analogy with Eq. (7.11).

Now the single grid points play the role of the cells in the continuous case. For each l, the approximate process starts with n_l particles in the grid point $l\sigma$. Its evolution is determined by the generator (7.1), (7.2), where the function h is replaced by (cf. (6.2), (6.1), (7.14)) $h_l(x, y) = 1$, the sum is taken over the appropriately reduced set of indices, and the coefficient B is chosen according to (7.10). Thus, the jump intensity is

$$\lambda_l = \frac{D n_l (n_l - 1)}{n\sigma^2}$$

Note that $|\mathscr{S}^0| = 2$. The expected number of jumps during a time interval of duration Δt is

$$\lambda_l \Delta t = \frac{D n_l (n_l - 1)}{n\sigma^2} \Delta t \tag{7.16}$$

Each jump consists of choosing a pair i, j, moving the first particle one step to the right and the second particle one step to the left, according to the transformation (7.2).

The corresponding approximate equations are obtained in analogy with (7.7), (7.8), and take the form

$$\frac{d}{ds}\,\tilde{p}_l(s, x) = Dp(t, l\sigma)\,\frac{\tilde{p}_l(s, x+\sigma) + \tilde{p}_l(s, x-\sigma) - 2\tilde{p}_l(s, x)}{\sigma^2}, \qquad s \geqslant t, \quad x \in G \tag{7.17}$$

with initial condition

$$\tilde{p}_l(t, x) = \chi_{\{l\sigma\}}(x)\; p(t, x), \qquad x \in G \tag{7.18}$$

and a recombination rule analogous to (7.9).

Remark 7.1. An explicit difference scheme for Eq. (7.15) provides

$$p(t + \Delta t, x) = p(t, x) + \Delta t\; D\,\frac{p(t, x+\sigma)^2 + p(t, x-\sigma)^2 - 2p(t, x)^2}{\sigma^2}, \qquad x \in G \tag{7.19}$$

Analogously, one obtains for Eqs. (7.17), (7.18)

$$\tilde{p}_l(t + \Delta t, x) = \tilde{p}_l(t, x) + \Delta t\; Dp(t, l\sigma) \times \frac{\tilde{p}_l(t, x+\sigma) + \tilde{p}_l(t, x-\sigma) - 2\tilde{p}_l(t, x)}{\sigma^2}, \qquad x \in G$$

which reduces to

$$\tilde{p}_l(t + \Delta t, l\sigma) = p(t, l\sigma) + \Delta t\; Dp(t, l\sigma)\,\frac{-2p(t, l\sigma)}{\sigma^2}$$

$$\tilde{p}_l(t + \Delta t, (l+1)\,\sigma) = \Delta t\; Dp(t, l\sigma)\,\frac{p(t, l\sigma)}{\sigma^2}$$

$$\tilde{p}_l(t + \Delta t, (l-1)\,\sigma) = \Delta t\; Dp(t, l\sigma)\,\frac{p(t, l\sigma)}{\sigma^2}$$

$$\tilde{p}_l(t + \Delta t, x) = 0, \qquad \text{otherwise}$$

Combining these equations via (7.9) one obtains

$$p(t+\Delta t, x) = p(t, x) + \Delta t\, Dp(t, x)\frac{-2p(t, x)}{\sigma^2} + \Delta t\, D\frac{p(t, x+\sigma)^2}{\sigma^2} + \Delta t\, D\frac{p(t, x-\sigma)^2}{\sigma^2}$$

$$= p(t, x) + \Delta t\, D\frac{p(t, x+\sigma)^2 + p(t, x-\sigma)^2 - 2p(t, x)^2}{\sigma^2}, \qquad x \in G$$

which is identical to (7.19).

Remark 7.2. In conclusion, the stochastic algorithm on the grid solves (as $n \to \infty$) Eq. (7.15), if there is an appropriate interaction between cell processes. This equation takes the form (7.12) when $\sigma \to 0$. The stochastic algorithm solves (as $n \to \infty$) Eqs. (7.17), (7.18), if there is no interaction between cell processes (this is the case for the original CBA). Here an additional Δt-error is involved. According to Remark 7.1, this limiting equation takes the form (7.15) when $\Delta t \to 0$, and therefore (7.12) when $\Delta t \to 0$, $\sigma \to 0$.

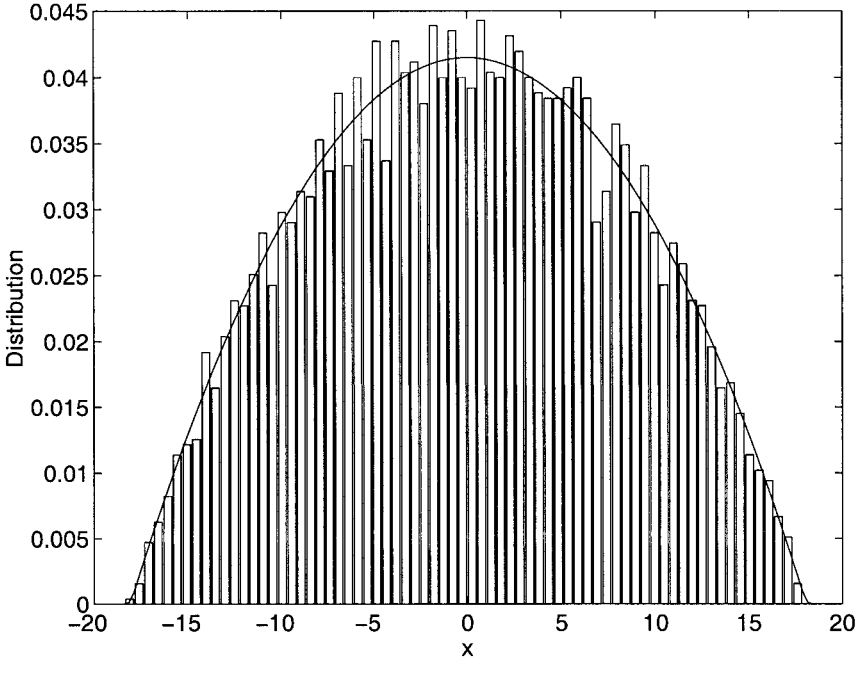

Fig. 2. Particle distribution in the stochastic system (histogram bars) and probability distribution from the explicit difference scheme (solid line) after 2^{15} time steps.

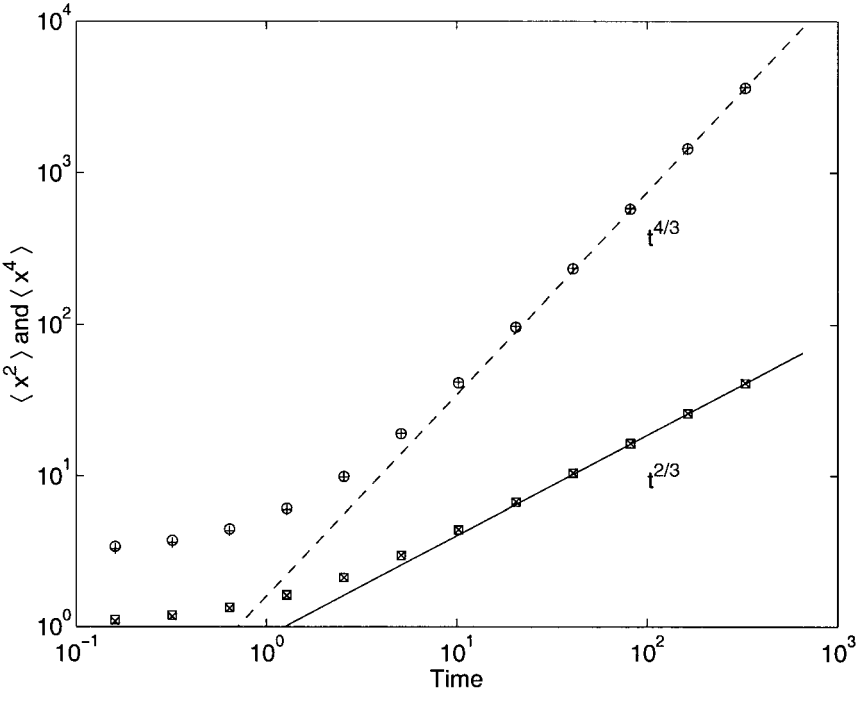

Fig. 3. Second and fourth moments versus time as measured in the stochastic system (□ and ○) and in the explicit difference scheme (× and +). The solid and dashed lines go as $t^{2/3}$ and $t^{4/3}$, respectively.

The results from numerical simulations of the stochastic system on a grid (cf. (7.16)) and of the explicit difference scheme (7.19) are shown in Figs. 2 and 3. The stochastic system has 5000 particles. For both the stochastic system and the difference scheme we take $\sigma = 0.3$, $D = 1$, and $\Delta t = 10^{-2}$. The initial distribution is a Gaussian with zero mean and unit variance; the distribution after a long time is bullet-shaped, as shown in Fig. 2. The second and fourth moments go as $t^{2/3}$ and $t^{4/3}$, as shown in Fig. 3; these results may be obtained from (7.12) using the scaling hypothesis (see appendix). Note that the distribution spreads more slowly than in the standard random walk model for which these moments go as t and t^2.

8. CONCLUDING REMARKS

The Consistent Boltzmann Algorithm has proven to be a useful computational tool in the study of moderately dense gases (see Section 1). The

algorithm's original formulation was based on general arguments from kinetic theory, specifically, considering how a displacement of colliding particles could give the hard-sphere virial. This paper gives CBA a better theoretical foundation by establishing the limiting kinetic equation for the stochastic process on which the numerical scheme is based. Many studies of this kinetic equation remain to be done: the proof of an H-theorem; the calculation of the equation of state and transport coefficients by the Chapman–Enskog expansion, etc. In brief, it will be of interest to repeat earlier studies that considered the Boltzmann and Enskog equations and, if these show the new kinetic equation to be fruitful, we will present them in a future paper.

APPENDIX: SCALING HYPOTHESIS FOR THE TOY MODEL

The scaling hypothesis states that the probability density scales as $p(x, t) = \alpha p(\alpha x, \alpha^a t)$, where the constant a is determined by the governing equation. For this equation we take the more general expression

$$\frac{\partial}{\partial t} p(x, t) = \frac{\partial^2}{\partial x^2} p^n(x, t)$$

with $n = 1$ giving the standard diffusion equation and $n = 2$ giving (7.12). To find the scaling power a, we define $z = \alpha x$, $s = \alpha^a t$ and write

$$\frac{\partial}{\partial t} p(x, t) = \alpha \frac{\partial}{\partial t} p(z, s) = \alpha^{a+1} \frac{\partial}{\partial s} p(z, s) = \alpha^{a+1} \frac{\partial^2}{\partial z^2} p^n(z, s)$$

$$= \alpha^{a-1} \frac{\partial^2}{\partial x^2} p^n(z, s) = \alpha^{a-1-n} \frac{\partial^2}{\partial x^2} p^n(x, t)$$

so $a = n + 1$. Now consider the moments of the distribution,

$$\langle x^m(t) \rangle = \int_{-\infty}^{\infty} x^m p(x, t)\, dx = \int_{-\infty}^{\infty} \alpha^{-m} z^m p(z, s)\, dz = \alpha^{-m} \langle x^m(s) \rangle$$

If the moments follow a power law of the form $\langle x^m \rangle \propto t^b$ then the scaling result gives $t^b = \alpha^{-m} (\alpha^a t)^b$ so $b = m/a$. For $n = 2$, the scaling power is $a = 3$ and $b = m/3$, in agreement with the results shown in Fig. 3.

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