CUBO A Mathematical Journal Vol. 9, № 1, (13 - 26). April 2007.

Global Solutions of the Enskog Lattice Equation with Square Well Potential

William Greenberg

Department of Mathematics, Virginia Tech, Blacksburg, Virginia 24061 USA greenberg@vt.edu

Michael Williams

Department of Mathematics, Virginia Tech, Blacksburg, Virginia 24061 USA williams@vt.edu

ABSTRACT

The nonlinear Enskog equation with a discretized spatial variable is studied in a Banach space of absolutely integrable functions of the velocity variables. The Enskog equation is a kinetic equation of Boltzmann type which, unlike the Boltzmann equation, is applicable to gases in the moderately dense regime. In this lattice model the generator of free streaming is replaced by a finite difference operator. Conservation laws and positivity are utilized to extend local solutions of a cutoff model to global solutions. Then compactness arguments lead to the existence of weak global solutions of the Enskog lattice equation. Molecular interactions are introduced via a next-nearest neighbor potential, thereby modeling a square well potential.

RESUMEN

La ecuación no lineal Enskog con la variable espacial discretizada se estudia en un espacio de Banach de funciones absolutamente integrables de las variables de velocidad. La ecuación de Enskog es una ecuación cinemática del tipo Boltzmann, la cual, no como la ecuación de Boltzmann, se aplica a gases en el régimen moderadamente denso. En el modelo de enrejado, el generador de fuente libre se reemplaza por un operador de diferencia finita. Las leyes de conservación y positividad se utilizan para extender las soluciones locales de un modelo de corte a soluciones globales. Luego, argumentos de de compacidad conducen a la existencia de soluciones globales débiles de la ecuación de enrejado Enskog. Las interacciones moleculares se introducen vía el potencial del vecino más cercano siguiente, luego modelando un potencial de pozo cuadrado.

> Key words and phrases: Math. Subj. Class.:

Enskog equation, kinetic theory, Boltzmann lattice 82C40, 76P05

1 Introduction

Although there is an extensive literature on discrete velocity Boltzmann equations, [1] and a smaller literature on discrete velocity Enskog equations.[2] the study of kinetic equations on spatially discrete domains is extremely limited. Here we would like to present a model of the Enskog equation on a three dimensional spatial lattice with the full velocity dependent Enskog collision operator. We will discuss as well a nextnearest neighbor interaction model which models the Enskog equation with square well potential, and, more generally, with local piecewise constant potential.

The Boltzmann equation, first posed in 1876, is the best known equation in the kinetic theory of gases.[3] However, this equation, which describes molecules as point particles and yields transport equations only of an ideal gas, is an accurate portrayal of a dilute gas. In order to have a more accurate description of moderately dense gases, Enskog in 1921 proposed the equation subsequently bearing his name.[4] The Enkog equation, revised in the 1960's to represent exact hydroynamics, takes into account the nonzero diameter of real molecules, and has turned out to be an accurate description of dense gases up to ten percent of close packing. Because the Enskog equation models only hard sphere collisions without intermolecular potential, Greenberg et al. have considered an Enkog type collision operator with square well, and, more generally, local picewise constant, potential [5, 6] Although discrete velocity models of the Boltzmann equation have an extens! ive literature going back more than 40 years, the spatially discrete Boltzmann equation was introduced more recently by Greenberg and coworkers.[7, 8] In these models the spatial variable is replaced by a finite periodic lattice.

In this article we will present a lattice version of the Enskog equation, studied in a Banach space of absolutely integrable functions of the velocity variables, i.e., only the spatial variable will be discretized. We will discuss both the analog of a hard sphere collision model and an Enskog model with local (next-nearest neighbor) interaction.

2 Streaming Lattice Operator

For perspective, let us write the Enskog equation in a three dimensional spatial domain:

$$\left[\frac{\partial}{\partial t} + \vec{v} \cdot \nabla_{\vec{r}}\right] f(\vec{r}, \vec{v}, t) = C_E(f, f)(\vec{r}, \vec{v}, t)$$
(2.1)

for a function $f : R^3_{\vec{r}} \times R^3_{\vec{v}} \times R_+ \to R_+$ representing the differential density of particles at position \vec{r} at time t with velocity \vec{v} . Here, $C_E(f, f)$ is the Enskog collision operator

$$C_E(f, f)(\vec{v}, \vec{v}, t) = \iint_{R^2 \times S_4^2} [Y(\vec{r}, \vec{r} + a\vec{\epsilon})f(\vec{r}, \vec{v}', t)f(\vec{r} + a\vec{\epsilon}, \vec{v}_1, t) \\ - Y(\vec{r}, \vec{r} - a\vec{\epsilon})f(\vec{r}, \vec{v}, t)f(\vec{r} - a\vec{\epsilon}, \vec{v}_1, t)] < \vec{\epsilon}, \vec{v} - \vec{v}_1 > d\vec{\epsilon} d\vec{v}_1, \quad (2.2) \\ \vec{v}' = \vec{v} - \vec{\epsilon} < \vec{\epsilon}, \vec{v} - \vec{v}_1 >, \quad \vec{v}_1' = \vec{v}_1 + \vec{\epsilon} < \vec{\epsilon}, \vec{v} - \vec{v}_1 >$$

for a gas of molecules of diameter a, with $\vec{\epsilon}$ -integration over $\{\vec{\epsilon} \in R^3 : ||\vec{\epsilon}|| = 1, \vec{\epsilon} \cdot (\vec{v} - \vec{v}_1) > 0\}$.

We shall consider the Enskog equation on a lattice:

$$\frac{\partial f_i}{\partial t}(\vec{v}, t) + (Af)_i(\vec{v}, t) = J(f, f)_i.$$
 (2.3)

The index *i* is the spatial index denoting the *i*th lattice point in the periodic threedimensional cubic lattice Λ^3 and \vec{v} is the (dimensionless) velocity vector. The operators *A* and *J* will be defined below. We seek solutions in the Banach space $\mathcal{X} = \bigoplus_i L^1(R^3)$ with norm $||f|| = \sum_i \int_{-\infty}^{\infty} |f_i(\vec{v})| d\vec{v}$, where the sums are over N^3 lattice sites. We denote with \mathcal{T}_+ the cone of positive functions in \mathcal{X} , and by $\mathcal{G}(\mathcal{I}_+)$ the cone of measurable functions $f(\cdot) : R_+ \to \mathcal{T}_+$.

The operator A with domain D(A) is the finite difference approximation to the gradient term. To give A specifically, let π be an identification between the lattice Λ^3 and Z^3 . Then A is an $\Lambda^3 \times \Lambda^3$ matrix:

$$A_{ij} = \sum_{\hat{u}} (\vec{v} \cdot \hat{u}) \Delta_{ij}^{\hat{u}}(\vec{v}) \qquad (2.4)$$

where

$$\Delta_{ij}^{\hat{u}}(\vec{v}) = \delta_{ij} - \delta_{i,\pi(\pi^{-1}(j)+\hat{u})}, \quad \vec{v} \cdot \hat{u} > 0, \quad \Delta^{\hat{u}}(-\vec{v}) = \Delta^{\hat{u}}(\vec{v}) *$$
(2.5)

and the sum is over the three orthogonal coordinate vectors \hat{u} . We have, for convenience, taken the lattice spacing to be of unit length. The periodic boundary conditions are imposed by viewing the lattice as a three-dimensional torus, and thus $\pi^{-1}(j) + \hat{u} \in \Lambda^3$ for every j.

A representation of A may be written as follows. If $v_x, v_y, v_z \geq 0$ and the $n \times n$ matrix E is defined by

$$E_{ij} = \begin{cases} \delta_{n,j}, & i = 1 \\ \delta_{i,j+1}, & i > 1 \end{cases}$$
(2.6)

OULEO

then

16

$$A = (v_x + v_y + v_z)I \otimes I \otimes I - v_x(E \otimes I \otimes I) - v_y(I \otimes E \otimes I) - v_z(i \otimes I \otimes E)$$
(2.7)

Note $E^n = I$ and that the representation of A if $v_i < 0$ can be obtained from 2.5. The discretized Enskog collision operator may be written

$$J(f, f)_i(\vec{v}, t) = G_0(f, f)_i(\vec{v}, t) - f_i(\vec{v}, t)L_0(f)_i(\vec{v}, t) =$$

$$\sum_{i \in \Gamma} \int_{R^3} d\vec{v}_1 \left[Y_{i,i+\epsilon} f_i(\vec{v}', t) f_{i+\epsilon}(\vec{v}'_1, t) - Y_{i,i-\epsilon} f_i(\vec{v}, t) f_{i-\epsilon}(\vec{v}_1, t) \right] \cdot$$

$$\cdot < \hat{\epsilon}, \vec{v} - \vec{v}_1 > \theta(\hat{\epsilon} \cdot (\vec{v} - \vec{v}_1)),$$
(2.8)

where θ is the Heaviside function and \vec{v}' , \vec{v}'_1 are given in 2.2. The geometric factor Y is a functional of f, $Y_{i,j} = Y(n_i(t), n_j(t))$, where $n_i(t) = \int_{R^3} d\vec{v} f_i(\vec{v}, t)$. The set $\Gamma \subset S^2$ is the set of unit vectors in R^3 pointing in the direction of nearest neighbors, taken periodically, eg., the unit coordinate vectors in a rectangular lattice. Indices such as $Y_{i,i+\epsilon}$ are written in shorthand for $Y_{i,\pi(\tau^{-1}(t)+t)}$.

Equation 2.3-2.8 is the discrete version of the (revised) Enskog equation 2.1, which models hard sphere collisions. The square well Enskog equation, derived by Davis et al.[9] and Greenberg et al.[5], models, in the continuum case, an intermolecular potential of the form

$$\phi(||\vec{r}_1 - \vec{r}_2||) = \begin{cases} \infty, & 0 < ||\vec{r}_1 - \vec{r}_2|| < a \\ -q, & a < ||\vec{r}_1 - \vec{r}_2|| < R \\ 0, & ||\vec{r}_1 - \vec{r}_2|| \ge R \end{cases}$$
(2.9)

for a single square well of depth q and width R, and a sequence of such wells for a piecewise constant local potential. The resultant kinetic equation has a collision term containing precisely the Enskog collision operator, on account of the hard sphere collision, and, in the case of a single square well, three very similar collision terms representing the molecule at $||\vec{r}_1 - \vec{r}_2|| = R$ (i) entering the well, (ii) exiting the well, and (iii) reflecting off the well if energy is not sufficient for an escape (or a penetration for a repulsive well). The last can not take place, of course, for an attractive well unless an intermediate collision has courred while the particle is in the well. In the case that the well consists of m piecewise constant steps, m_1 attractive transitions, and m_2 repulsive transitions, the collision operator will contain $3m_1 + 2m_2 + 1$ Enskog-like collision

As we are interested in lattice models, we will defer writing out the continuum equation for square well potentials, recommending the reader to the quoted literature, and restrict ourselves to writing the lattice equation. In the case of a single well, which translates into a strictly next-nearest neighbor interaction, the lattice collision operator is:

$$J(f,f)_{i}(\vec{v},t) = \sum_{\vec{e}\in\Gamma_{0}} \int_{R^{3}} d\vec{v}_{1} \left[Y_{i,i+\epsilon} f_{i}(\vec{v}',t) f_{i+\epsilon}(\vec{v}_{1},t) - Y_{i,i-\epsilon} f_{i}(\vec{v},t) f_{i-\epsilon}(\vec{v}_{1},t) \right].$$



Enskog Lattice Equation with Square Well

$$\hat{\epsilon} \cdot (\vec{v} - \vec{v}_1)\theta(\hat{\epsilon} \cdot (\vec{v} - \vec{v}_1)) +$$
 (2.10)

$$\begin{split} + \sum_{\epsilon \in \Gamma_1} \int_{R^3} d\vec{v}_1 \left[Y_{i,i+\epsilon} f_i(\vec{v}'',t) f_{i+\epsilon}(\vec{v}_1'',t) - Y_{i,i-\epsilon} f_i(\vec{v},t) f_{i-\epsilon}(\vec{v}_1,t) \right] \cdot \\ \cdot \hat{\epsilon} \cdot (\vec{v} - \vec{v}_1) \theta(\hat{\epsilon} \cdot (\vec{v} - \vec{v}_1)) + \\ + \sum_{\epsilon \in \Gamma_1} \int_{R^3} d\vec{v}_1 \left[Y_{i,i-\epsilon} f_i(\vec{v}'',t) f_{i-\epsilon}(\vec{v}_1'',t) - Y_{i,i+\epsilon} f_i(\vec{v},t) f_{i+\epsilon}(\vec{v}_1,t) \right] \cdot \end{split}$$

$$\hat{\epsilon} \cdot (\vec{v} - \vec{v}_1)\theta(\hat{\epsilon} \cdot (\vec{v} - \vec{v}_1) - \sqrt{4q}) +$$

$$\begin{split} &+ \sum_{\epsilon \in \Gamma_1} \int_{R^3} d\vec{v}_1 \left[Y_{i,i-\epsilon} f_i(\vec{v}',t) f_{i-\epsilon}(\vec{v}_1',t) - Y_{i,i+\epsilon} f_i(\vec{v},t) f_{i+\epsilon}(\vec{v}_1,t) \right] \cdot \\ & \cdot \theta(\sqrt{4q} - \hat{\epsilon} \cdot (\vec{v} - \vec{v}_1)) \hat{\epsilon} \cdot (\vec{v} - \vec{v}_1) \theta(\hat{\epsilon} \cdot (\vec{v} - \vec{v}_1)) = \\ &= \sum_{k=0}^3 [G_k(f,f)_i - f_i L_k(f)_i] = G(f,f)_i - f_i L(f)_i, \end{split}$$

where Γ_0 is the set of nearest neighbor vectors and Γ_1 is the set of next-nearest neighbor vectors. Here, the double and triple primed velocities are derived by conservation of momentum and energy, just as were the velocity transformations in 2.2. For example,

$$\vec{v}'' = \vec{v} - \frac{1}{2}\vec{\epsilon}\{<\vec{\epsilon}, \vec{v} - \vec{v}_1 > -[<\vec{\epsilon}, \vec{v} - \vec{v}_1 >^2 + 4q]^{\frac{1}{2}}\},\tag{2.11}$$

$$\vec{v}_1'' = \vec{v}_1 + \frac{1}{2}\vec{\epsilon}\{<\vec{\epsilon}, \vec{v} - \vec{v}_1 > -[<\vec{\epsilon}, \vec{v} - \vec{v}_1 >^2 + 4q]^{\frac{1}{2}}\},\tag{2.12}$$

with a similar transformation for $\vec{v}^{\prime\prime\prime}$, $\vec{v}_{1}^{\prime\prime\prime}$. (cf. [3]).

In the case of next⁴-nearest neighbor interactions for $i = 1, \cdots, m$, there will be additional collision terms as indicated for the continuum equation with corresponding transformations of (primed) outgoing velocities, obtained by the conservation laws and taking into account the energy levels q_i . In this case, there will be summations over next⁴-nearest neighbor vectors Γ_i and $J(f, f) = \sum_{i=0}^{2m_i+3m_i} [\sigma_{\mathbf{k}}(f, f) - fL_{\mathbf{k}}(f)]$. As the functional analysis to be considered in what follows carries over in a transparent way to these additional collision terms, we will, for convenience, pose the lemmas for the case of nearest neighbor interaction only, i.e., the lattice collision operator 2.8, commenting only on any issues for which the lattice model with interaction potential might differ.

3 Semigroup and Iterations

We assume that Y is positive, symmetric, bounded and jointly continuous in its arguments, with the conservation (of mass) property

$$\int_{R^3} d\vec{v} \{ G(f,f)_i - f_i L(f)_i \} = 0, \quad f \in \mathcal{X}.$$
(3.1)

Throughout this and the following section, we will consider only the velocity cutoff model, which includes in the collision kernel the additional factor $\theta(p - ||\vec{v} - \vec{v}_1||)$ for some fixed p > 0. Then G and L are bounded functionals: $||G(f, f)|| \le k_1 ||f||^2$ and $||L(f)|| \le k_2 ||f||$ for constants k_1, k_2 depending on p.

Throughout, we will suppress the position variable (index) when the meaning remains clear.

It is easy to see that A generates a c_0 -semigroup $U_A(t)$ and A + L(f) a twoparameter evolution operator T_f , ie, $T_f(t, s)\xi_0$ is a solution of the homogeneous equation

$$\frac{dg}{dt} + Ag + L(f)g = 0, \qquad g(s) = \xi_0.$$
(3.2)

We consider the integral equation

$$f(t) = U_A(t)f_0 + \int_0^t ds \, U_A(t-s) \{ G(f(s), f(s)) - f(s)L(f(s)) \}$$
(3.3)

as well as the equation

$$f(t) = T_f(t,0)f_0 + \int_0^t ds \, T_f(t,s)G(f(s),f(s)).$$
(3.4)

Note that for next-nearest neighbor interactions, the integral in 3.4 will be

$$\int_{0}^{t} ds T_{f}(t,s) \sum_{k=0}^{3m} G_{0}(f(s),f(s)).$$
(3.5)

Lemma 3.1

- (a) U_A(t) and T_f(t₂,t₁) are invariant on the cone of positive functions T₊ ⊂ X for t and t₂ − t₁ positive, and f ∈ G(T₊).
- (b) U(t) is a contraction semigroup and continues analytically to a bounded holomorphic semigroup U(z).
- (c) $T_f(t_2, t_1)$ is a contraction mapping on \mathcal{X} for $t_2 t_1$ positive and $f \in \mathcal{G}(\mathcal{T}_+)$.

Proof. Let M_N denote the union of subspaces of functions of T_+ with support in the hypercube about the origin with sides of length 2N. Since the off-diagonal terms of U_A are positive for any $-A^l$, if $(-A^m)_{ki} = 0$, $m \leq l$, then $(-A^{l+1})_{ki} \geq 0$. Therefore, every element of e^{-tA} is a power series in $t|\vec{v} \cdot \hat{u}|$ with positive coefficient to



lowest order. Hence, for $t|\vec{v} \cdot \hat{u}|$ sufficiently small, $(e^{-tA}f)_t \ge 0$ for $f \in \mathcal{T}_+ \cap M_N$. By exponential addition, this extends to aritrary t. Therefore $U_A(t)\mathcal{T}_+ \cap M_N \subset \mathcal{T}_+ \cap M_N$, and $U_A(t)\mathcal{T}_+ \subset \mathcal{T}_+$.

On M_N , $\mathcal{A}(t) = -A - L(f(t))$ is a bounded operator, and $T_f(s, t)$ is given explicitly by

$$T_f(t,s) = \operatorname{s.\lim}_{m \to \infty} \exp \int_{t_{m-1}}^{t_m} \mathcal{A}(t') dt' \exp \int_{t_{m-2}}^{t_{m-1}} \mathcal{A}(t') dt' \dots \exp \int_{t_0}^{t_1} \mathcal{A}(t') dt' \quad (3.6)$$

with the limit taken over *n*-partitions $t = t_m > t_{m-1} > \cdots > t_1 > t_0 = s$. Using the Lie product formula and the uniform boundedness of each of the exponentials, one can represent $\Gamma_t(t, s)$ as the double limit

$$T_{f}(t,s) = s \lim_{m \to \infty} \lim_{n \to \infty} \left\{ \left[U_{A} \left(\frac{t_{m} - t_{m-1}}{n} \right) \exp \frac{-\int_{t_{m-1}}^{t_{m}} L(f(s)) ds}{n} \right]^{n} \cdot \left\{ U_{A} \left(\frac{t_{1} - t_{0}}{n} \right) \exp \frac{-\int_{t_{0}}^{t_{1}} L(f(s)) ds}{n} \right]^{n} \right\}$$
(3.7)

But L is diagonal and positive on \mathcal{T}_+ , and therefore so are the exponentials in 3.7. Thus $T_f(t,s)\mathcal{T}_+ \subset \mathcal{T}_+$, completing the proof of (a).

To prove (b), note that $\sum_{i=1}^{N^3} (A^m)_{ij} = 0$ for any $m \in \mathbb{Z}_+$. By a simple computation, $U_A(t)$ is seen to be isometric on \mathcal{I}_+ . But a \mathcal{I}_+ -invariant contractive linear map is contractive on \mathcal{X} , so $U_A(t)$ is contractive on \mathcal{X} .

To prove $U_A(t)$ extends to a bounded holomorphic semigroup, consider first the case $v_i > 0$. Denote $E_0 = I$, $E_1 = E$ and $E_\alpha = E_{\alpha-1}E$. Then $E_{n+\alpha} = E_\alpha$. Therefore,

$$e^{sE} = \sum_{\alpha=0}^{n-1} \left(\sum_{p=0}^{\infty} \frac{s^{np+\alpha}}{(np+\alpha)!} \right) E_{\alpha} = \sum_{\alpha=0}^{n-1} h_{\alpha}(s) E_{\alpha}.$$
 (3.8)

Let w_{α} be the primitive nth roots of unity. Then $e^{sw}\alpha = \sum_{\beta=0}^{n-1} h_{\beta}(s)w_{\alpha}$. Substituting into 3.8, one has $h_{\alpha}(s) = \frac{1}{n} \sum_{i=1}^{n} w_{-\alpha i} e^{sw_i}$, so

$$e^{s(-I+E)} = \frac{1}{n} \sum_{\alpha=0}^{n-1} \sum_{i=1}^{n} e^{s(w_i-1)} w_{-\alpha i} E_{\alpha}.$$
(3.9)

Writing $U_A(s) = U_x(s) \otimes U_y(s) \otimes U_z(s)$, to show $U_A(s)$ is a bounded holomorphic senigroup, it is sufficient to show that $U_x(s)$ and $sAU_x(s)$ are bounded uniformly in a sector $S_g \subset C$,

$$\mathcal{S}_{\theta} = \{ z \in C | | \arg z | < \theta < \frac{\pi}{2} \}.$$
(3.10)

Then from the above, if s = u + iv and $w_i = \cos\theta_i + i\theta_i$, $U_x(s)$ will be uniformly bounded for

$$\frac{u}{v} \ge \frac{\sin \theta_i}{\cos \theta_i - 1} = -\cot \frac{\theta_i}{2},\tag{3.11}$$



19

an inequality which can always be satisfied for positive u. A similar computation for $v_x < 0$ shows the uniform boundedness of $U_A(t)$. The uniform boundedness of sAU(s) is an immediate consequence of the boundedness of $g(\xi) = \xi e^{-\xi}$, $Re \ \xi \ge 0$. This proves (b).

Finally, since L is positive, $\exp\{-\int ds L(f(s))\}$ is contractive, and by the representation 3.7, part (c) is proved, completing the proof of the theorem.

Lemma 3.2 For all $f \in \mathcal{X}$,

$$\sum_{i=1}^{N^3} (U(t)f)_i = \sum_{i=1}^{N^3} f_i.$$
(3.12)

OUIBL

Let us solve 3.3 by iteration. Define

$$f^{(0)}(\vec{v}, t) = f_0(\vec{v})$$
 (3.13)

$$f^{(n)}(\vec{v},t) = U_A(t)f_0(\vec{v}) + \int_0^t ds \, U_A(t-s)J(f^{(n-1)},f^{(n-1)})(s) \tag{3.14}$$

Lemma 3.3 For t sufficiently small, $||f^{(n)}|| \leq M$, independent of t and n, and

$$|f^{(n+1)} - f^{(n)}|| \le t ||J(f^{(n)}, f^{(n)}) - J(f^{(n-1)}, f^{(n-1)})||$$

$$\le 2tM ||J||||f^{(n)} - f^{(n-1)}||.$$
(3.15)

The lemma follows from the boundedness of the collision operator. Thus,

Lemma 3.4 The iterative scheme 3.14 converges to a solution f(t) of 3.3 for

$$t < \min\{\frac{1}{4||J|||f_0||}, \frac{1}{2||J||M}\},$$
(3.16)

and f(t) is a continuous function of the initial datum f_0 .

Next define the iterative scheme

$$g^{(0)}(\vec{v},t) = f_0(\vec{v})$$
 (3.17)

$$g^{(n+1)}(\vec{v},t) = T_{g^{(n)}}(t,0)f_0(\vec{v}) + \int_0^t ds \, T_{g^{(n)}}(t,s)G(g^{(n)}(s),g^{(n)}(s))$$
(3.18)

As before, we have

Lemma 3.5 For t sufficiently small, $||g^{(n)}(t)|| \le M_1$ and $\{g^{(n)}(t)\}$ is Cauchy.

Proof. To see the sequence is Cauchy, define

$$g^{(n+\frac{1}{2})}(\vec{v},t) = T_{g^{(n-1)}}(t,0)f_0(\vec{v}) + \int_0^t ds \, T_{g^{(n-1)}}(t,s)G(g^{(n)}(s),g^{(n)}(s)) \tag{3.19}$$



and write S_s^t for $\sup_{0 \le s \le t}$. Then we have easily from Lemma 3.1,

$$||g^{(n+\frac{1}{2})}(t) - g^{(n)}(t)|| \le 2t||G||M_1S_s^t||g^{(n)}(s) - g^{(n-1)}(s)||$$
(3.20)

for t sufficiently small. Again from Lemma 3.1,

$$||g^{(n+1)}(t) - g^{(n+\frac{1}{2})}(t)|| \le ||T_{g^{(n)}}(t,0) - T_{g^{(n-1)}}(t,0)||||f_0|| +$$
(3.21)

 $+t||G||S_s^t||T_{g^{(n)}}(t,s) - T_{g^{(n-1)}}(t,s)||||g^{(n)}(s)||^2.$

Define $\chi(t)=(T_{g^{(n)}}(t,s)-T_{g^{(n-1)}}(t,s))\xi_0$ for fixed s. Then χ is the solution of the coupled system

$$\frac{dg}{dt} + [A + L(g^{(n)}(t))]g = 0, \qquad g(s) = \xi_0$$
(3.22)

$$\frac{d\chi}{dt} + [A + L(g^{(n-1)}(t))]\chi = L(g^{(n-1)}(t) - g^{(n)}(t))g(t), \qquad \chi(s) = 0.$$
(3.23)

Then from

$$\chi(t) = \int_0^t ds \, T_{g^{(n)}}(t,s) L(g^{(n-1)}(s) - g^{(n)}(s))g(s) \tag{3.24}$$

we have

$$||g^{(n+1)}(t) - g^{(n+\frac{1}{2})}(t)|| \le ||L||(t||f_0|| + t^2||G||M_1^2)S_s^t||g^{(n)}(s) - g^{(n-1)}(s)||$$
(3.25)

Collecting these results, it is sufficient to assume $0 \le t \le T_0$ for $T_0^{-1} = 8||G||M_1 + 8M_1 + 5||L||||f_0||$ to obtain

$$||g^{(n+\frac{1}{2})}(t) - g^{(n)}(t)|| \le \frac{1}{4}S^t_s||g^{(n)}(s) - g^{(n-1)}(s)||$$
(3.26)

$$||g^{(n+1)}(t) - g^{(n+\frac{1}{2})}(t)|| \le \frac{1}{4}S_s^t||g^{(n)}(s) - g^{(n-1)}(s)||.$$
 (3.27)

From the estimates it is evident that the sequence $\{g^{(n)}\}$ is Cauchy.

Lemma 3.6 Define $g^{(n)}(\vec{v}, t)$ by the iterative scheme 3.18. Then for t sufficiently small, $g^{(n)}(t)$ converges in X to g(t), and g is a solution of 3.4.

Lemma 3.7 $g(t) \in T_+$.

4 Global Solutions

We will extend the mild local solutions of Section 3 to global-in-time solutions, and then prove they are classical solutions (for the velocity cutoff model).

Lemma 4.1 Let g_1 , g_2 be solutions of 3.3,3.4, respectively, satisfying $g_1(0) = g_2(0) = f_0$. Then $g_1 = g_2$.



OUEO

Proof. One can compute from 3.4

$$g_2(t + s) =$$
 (4.1)

$$\begin{split} T_{g_2}(t+s,t) \big[T_{g_2}(t,0) f_0 + \int_0^t dt' \, T_{g_2}(t,t') G(g_2(t')) \big] + \int_t^{t+s} dt' \, T_{g_2}(t+s,t') G(g_2(t')) = \\ T_{g_2}(t+s,t) [g_2(t) + s G(g_2(t)) + O(s)]. \end{split}$$

Define $\eta(s) = [T_{g_2}(t+s,t) - U(s)]\xi_0$. From

$$\frac{\partial \eta}{\partial s} = -[A + L(g_2(t+s))]\eta(s) - L(g_2(t+s))U_A(s)\xi_0$$
(4.2)

and $\eta(0) = 0$, we have

$$\eta(s) = -\int_0^s dt' T_{g_2}(t+s,t+t') L(g_2(t+t')) U_A(t')\xi_0.$$
(4.3)

Combining this with 4.1, we may write

$$g_2(t+s) = U_A(s)[g_2(t) + sG(g_2)) - sL(g_2(t))g_2(t)] + O(s).$$
(4.4)

On the other hand,

$$g_{1}(t+s) = U_{A}(s)U_{A}(t)f_{0} + \int_{0}^{t} dt' U_{A}(s)U(t-t')J(g_{1}(t'),g_{1}(t')) +$$

$$+ \int_{t}^{t+s} U_{A}(t+s-t')J(g_{1}(t'),g_{1}(t'))$$

$$= U_{A}(s)[g_{1}(t) + sJ(g_{1}(t),g_{1}(t))] + O(s)$$

$$(4.5)$$

Writing $\alpha(t) = ||g_2(t) - g_1(t)||$, we have

$$\alpha(t+s) - \alpha(t) \le s||J||(||g_2(t)|| + ||g_1(t)||)||g_2(t) - g_1(t)||$$

$$(4.6)$$

or

$$\mathcal{D}^{+}\alpha(t) \le 2||J||\alpha(t) \sup_{i,0 \le t \le T_0} ||g_i(t)||.$$
(4.7)

The Gronwall Lemma completes the proof.

We wish to show that the solution of 3.3 is differentiable in t, and thus a solution of 2.3. Since $U_A(t)$ is a holomorphic semigroup, it is sufficient, by Kato's theorem, to show that J(f(t), f(t)) is Hölder continuous. [10, pp. 487-491] This will follow from the Hölder continuity of f(t).

Lemma 4.2 For $f_0 \in \mathcal{T}_+ \cap \mathcal{D}(A)$, $\{f^{(n)}(t)\}$ given by the iterative scheme 3.14 are differentiable on some interval $[0, T_0]$, and the derivatives $\{f^{(n)}(t)\}$ are uniformly bounded in t and n.



0, 1(2007

Proof. Estimate

OUR

$$f^{(n)}(t+h) - f^{(n)}(t) = (U_A(h) - I) \bigg\{ U_A(t) f_0 +$$
(4.8)

$$+ \int_0^t dt' U_A(t-t') [J(f^{(n-1)}(t'), f^{(n-1)}(t')) - J(f^{(n-1)}(t), f^{(n-1)}(t))] + \\ + \int_0^t dt' U_A(t-t') J(f^{(n-1)}(t), f^{(n-1)}(t)) \bigg\} + h U_A(h) J(f^{(n-1)}(t), f^{(n-1)}(t)) + O(h)$$

Therefore, the right derivative is

$$D^+g^{(n)}(t) = AU_A(t)f_0 +$$
 (4.9)

$$+A[\int_0^t U_A(t-t')J(f^{(n-1)}(t'),f^{(n-1)}(t'))] + U_A(t)J(f^{(n-1)}(t),f^{(n-1)}(t)).$$

Then a bound on $\mathcal{D}^+f^{(n)}(t)$ is obtained by the estimate $||AU_A(t)|| \leq K/t$ for some constant K (by analyticity). In particular, for $n \geq 2$,

$$||\mathcal{D}^+g^{(n)}(t)|| \le ||Af_0|| + tK||J||2m\frac{||f^{(n-1)}(t') - f^{(n-1)}(t)||}{t' - t} + ||J||m^2$$
(4.10)

and a uniform bound is obtained inductively by estimating Lipschitz constants K_n for each $f^{(n)}$. Indeed, for n = 1, $\mathcal{D}^+f^{(1)}(t) = U_A(t)Af_0 + U_A(t)J(f_0, f_0)$ and $f^{(1)}$ is Lipschitz with constant $K_1 = ||Af_0|| + ||J|||f_0||^2$. and for $n \ge 2$ from the estimate above we have

$$||f^{(n)}(t) - f^{(n)}(s)|| \le (||Af_0|| + ||J||m^2 + 2tKm||J||K_{n-1})|t - s|,$$
(4.11)

so that

$$K_n = \alpha + t\beta K_{n-1} \tag{4.12}$$

with $\alpha = ||Af_0|| + ||J||m^2$ and $\beta = 2Km||J||$, which is uniformly bounded for t < 1/(2Km||J||). This completes the proof

Lemma 4.3 The $\{f^{(n)}(t)\}$, as specified by the iterative scheme 3.14, are Lipschitz with a uniform Lipschitz constant $K = \alpha(1 - T_0\beta)^{-1}$ for $t < T_0$.

Lemma 4.4 For $f_0 \in T_+ \cap D(A)$, the solution of 3.3 is differentiable, and therefore a solution of 2.3, for $t < T_0$

Theorem 4.1 Suppose $f_0 \in T_+ \cap D(A)$. Then there exists a unique positive solution f(t) of the integral equation 3.3, or equivalently 3.4, for all $t \ge 0$, and f(t) is a continuously differentiable solution of the Enskog lattice equation 2.3 for the velocity cutoff model. Further, $f(t) \in T_+$ and f depends continuously upon the initial datum f_0 .

Proof. It remains only to note that $||f(t)|| = ||f_0||$ for t sufficiently small. For, integrating 3.3 over \vec{v} and summing over i, recalling $U_A(t)$ is an isometry on T_+ , we have (for t sufficiently small)

$$||f|| = ||f_0|| + \sum_{\hat{u} \in \Gamma} \int_{R^3} d\vec{v} \int_0^t ds \sum_{i=1}^{N^3} [U_A(s)J(f(s), f(s))]_i.$$
(4.13)

Using Lemma 3.2, this becomes

$$||f|| = ||f_0|| + \int_0^t ds \sum_{i=1}^{N^3} \sum_{\ell \in \Gamma} \int_{R^3} d\vec{v} \left[J(f(s), f(s)) \right]_i.$$
(4.14)

But 1 is a collision invariant. Hence the integral term vanishes, and $||f|| = ||f_0||$. Now, the procedure can be repeated, and the theorem follows.

Note that the theorem is valid both for the lattice system with (cutoff) Enskog collision operator and with next^m-nearest neighbor interaction for any m < N.

5 Removal Of The Cutoff

Finally, let us consider the lattice model 2.3 with next¹-nearest neighbor interaction (without cutoff). We continue to suppress the spatial index *i* when possible. We assume given an initial distribution on the lattice $f_0(\vec{v})_i \in T_+$ with finite mass, energy and entropy:

$$\sum_{i} \int_{R^{3}} d\vec{v} f_{0}(\vec{v})_{i} \{1 + v^{2} + |\log f_{0}(\vec{v})_{i}|\} < \infty.$$
(5.1)

By the results of section 4, for each positive integer p, the cutoff lattice equation 2.3 has a classical solution $f^{(p)}(\vec{v}, t)_i$, satisfying $f^{(p)}(\vec{v}, 0)_i = f_0(\vec{v})_i$. Fix a time interval [0, 7]. Then, for these solutions, the equality

$$\sum_{i} \int_{R^3} d\vec{v} f^{(p)}(\vec{v}, t)_i = \sum_{i} \int d\vec{v} f^{(p)}(\vec{v}, 0)_i$$
(5.2)

and estimate

$$\sum_{i} \int_{\mathbb{R}^{3}} d\vec{v} \, v^{2} f^{(p)}(\vec{v}, t)_{i} \leq k_{1} \sum_{i} \int_{\mathbb{R}^{3}} d\vec{v} \, v^{2} f^{(p)}(\vec{v}, 0)_{i} + k_{2}$$
(5.3)

for $t \in [0, T]$ and constants k_1, k_2 depending on T are a result of the symmetry of the collision kernel (cf. [6]).

Lemma 5.1 $H(f^{(p)}(\vec{v},t)) \leq H(f^{(p)}(\vec{v},0)) + k_3$, where

$$H(f) = \sum_{i} \int_{R^{3}} d\vec{v} f(\vec{v})_{i} \log f(\vec{v})_{i}$$
(5.4)

and k_3 is a function of T and $f_0(\vec{v})$.

Proof. Since $U_A(t)_{ij} \ge 0$ and $\sum_i U_A(t)_{ij} = 1$ by the proof of Lemma 3.1, then for fixed velocity $\vec{v}, U_A(t)$ is the transition matrix for a discrete Markov system. Since any space-independent distribution is a fixed point of $U_A(t)$, standard arguments [11] prove that $H(U_A(t)f_0(\vec{v})_i)$ is nonincreasing. Now the lemma follows from estimates in [6].

Theorem 5.1 Suppose $\sum_i \int_{R^3} d\vec{v} f_0(\vec{v})_i \{1 + v^2 + |\log f_0(\vec{v})_i|\} < \infty$ and $f^{(p)}(\vec{v}, t)_i$ is a solution of the lattice equation with cutoff p and $f^{(p)}(\vec{v}, 0)_i = f_0(\vec{v})_i$. Then $\{f^{(p)}\}$ contains a subsequence which converges weakly in χ . The limit function $f(\vec{v}, t)_i$ is continuous in t and satisfies the integral equation 3.3 with unbounded collision kernel.

Proof. The Dunford-Pettis property of L^1 and the mass, energy, entropy bounds previously demonstrated prove the existence of a subsequence (as $p \to \infty$) converging weakly in χ to a function f(t) for a demunerable dense set of t. Extension to all t follows from the equicontinuity of the family $\{f^{(p)}\}$. Indeed, let $\chi_v = \{f \in \chi :$ $(1+v^2)^{\frac{1}{2}}f((\tilde{v}) \in \chi)$. Since $f^{(p)}$ is a solution of 2.3, $||f^{(p)'}(t)|| \le ||A_f^{(p)}(t)|| + K||f^{(p)}||_v^2$, with K independent of p. Further, $||A_f^{(p)}|| \le 6||f^{(p)}||_v$. Then using $||f^{(p)}||_v \le ||f_0||_v$, equicontinuity of the sequence follows.

Since χ_v also satisfies the Dunford-Pettis property, and $J: \chi_v \times \chi_v \to \chi$ is weakly continuous, $J(f^{(p)}(t))$ converges weakly to J(f(t)) pointwise in t. Then, using the integral equation for $f^{(p)}$, the dominated convergence theorem, and the continuity of J, one can see that the limit function f(t) satisfies equation 3.3.

Again, the result is equally valid for the Enskog lattice equation and for the lattice equation with nextⁱ-nearest neighbor interaction. The cost of treating the equation without velocity cutoff is the weakness of the solution and the loss of a uniqueness proof.

Received: Sep 2005. Revised: Oct 2005.

References

- R. GATIGNOL, Theorie Cinetique de Gaz a Repartition Discrete de Vitesses, Lecture Notes in Phys. 36, Springer-Verlag, New York, 1975.
- [2] G.TOSCANI, On the discrete velocity models of the Boltzmann equation in several dimensions, Ann. Matem. Pura Appl. 138, (1984) 279–308.
- [3] C. CERCIGNANI, Theory and Application of the Boltzmann Equation, Elsevier, New York, 1978.
- [4] N. BELLOMO, M. LACHOWICZ, J. POLEWCZAK AND G. TOSCANI, Mathematical Topics in Nonlinear Kinetic Theory II: the Enskog Equation, World Scientific, London, 1991.



CUBO

- [5] W. GREENBERG, P. LEI AND R.S. LIU, Stability theory for the kinetic equations of a moderately dense gas, in Rarefied Gas Dynamics: Theory and Simulations (Progress in Astronautics and Aeronautics, vol. 159), B.D. Shizgal and D.P. Weaver, eds., American Inst. Aeron. Astron., Washington, DC, 1994, pp. 599–607.
- [6] W. GREENBERG AND A. YAO, Kinetic equations for gases with piecewise constant intermolecular potentials, Transport Theory and Stat. Phys. 27, (1997) 137–150.
- [7] C. CERCIGNANI, W. GREENBERG AND P.F. ZWEIFEL, Global solutions of the Boltzmann equations on a lattice, J. Stat. Phys. 20, (1979) 449–462.
- [8] W. GREENBERG, J. VOIGT AND P.F.ZWEIFEL, Discretized Boltzmann equation: lattice limit and non-Maxwellian gases, J. Stat. Phys. 21, (1979) 649–657.
- [9] H.T. DAVIS, S.A. RICE AND J.V. SENGERS, On the kinetic theory of dense fluids. IX, the fluid of rigid sphere well attraction, J. Chem. Phys. 35, 2210 (1961).
- [10] T. KATO, Perturbation Theory for Linear Operators, Springer, New York, 1966.
- M. MOREAU, Note on the entropy production in a discrete Markov system, J. Math. Phys. 19, (1978) 2494–2498.