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Discretized Boltzmann Equation: Lattice Limit and Non-Maxwellian Gases

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We continue the study of a discrete model of the Boltzmann equation, in which the spatial variable is replaced by a finite periodic lattice. Using a weak compactness criterion for L_1, the existence of a lattice limit as the lattice spacing tends to zero is proved. The case of unbounded collision kernels (non-Maxwellian gases) is also treated.

KEY WORDS: Boltzmann equation; finite-difference approximation; lattice limit; global solutions; non-Maxwellian gases.

1. INTRODUCTION

In a recent paper,[1] an existence and uniqueness theorem was proved for a special model of the Boltzmann equation. The major attribute of the model was a lattice representation of the Boltzmann equation, i.e., the spatial variable was replaced by a discrete set of points and the spatial gradient by a suitable difference formula. In addition, the collision kernel was taken to be that for a "cutoff" Maxwell gas.[2] (Spohn[3] has also treated the same problem in a slightly different way.)

The purpose of this paper is to prove the existence of a weak limit to the solutions of the latticized equations as the lattice spacing tends to zero and to relax the Maxwell gas collision assumption. Some of the results have been announced previously[4]; here we present the proofs.

The basic idea is to restrict the initial data to finite energy and entropy. We are then able to show (Section 2) that the lattice approximation conserves

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energy and satisfies an H theorem with the (increasing) entropy and the energy uniformly bounded with respect to the lattice spacing. This, in turn, enables us to apply a weak compactness criterion and demonstrate the existence of a weak limit (Section 3), employing techniques similar to those used by Morgenstern[5] and Arkeryd.[6] The extension to more general collision models than the Maxwell gas follows from similar arguments (Section 4). We point out that it is not known under what conditions (if any) on the collision operator the weak limit is a solution, in some sense, of the original Boltzmann equation.

2. PROPERTIES OF THE MODEL

We repeat some of the notation introduced in Refs. 1 and 4, for the reader's convenience. The Boltzmann equation is treated in the real Banach space

$$B^n = L_1(\Gamma_n \times \mathbb{R}^3)$$

with norm

$$\|f\|_{B^n} = 2^{-3n} \sum_{i \in \Gamma_n} \int_{\mathbb{R}^3} |f_i(c)| \, dc$$

Here, $\Gamma_n = \{1 \cdot 2^{-n}, 2 \cdot 2^{-n}, \ldots, 2^n \cdot 2^{-n}\}^3$ is a discrete set with cardinality 2^{3n}, representing a lattice approximation to the continuum $\Gamma = [0, 1]^3$, with lattice spacing 2^{-n}. We shall also utilize the subspace $B_\kappa{}^n \subset B^n$ defined as

$$B_\kappa{}^n = \{f \in B^n | (1 + c^2)^{\kappa/2} f \in B^n\}$$

with norm

$$\|f\|_\kappa = \|(1 + c^2)^{\kappa/2} f\|_{B^n}$$

The variable c represents the velocity, while the subscript i refers to the ith lattice point. We visualize the lattice Γ_n as a three-dimensional cubical array, with periodic conditions imposed on the boundaries, in accord with the finite-difference approximation to the gradient implicit in the definition of A^n given below.

The gradient term of the Boltzmann equation is, in the spirit of the lattice approximation, replaced by a finite-difference approximation A^n. Thus

$$2^{-n}(A_x{}^n f)_{(j,k,l)} = \begin{cases} c_x(f_{(j,k,l)} - f_{(j-2^{-n},k,l)}), & c_x > 0 \\ c_x(f_{(j+2^{-n},k,l)} - f_{(j,k,l)}), & c_x < 0 \end{cases}$$

and with similar expressions for $A_y{}^n$ and $A_z{}^n$, and A^n is obtained from $A_x{}^n$, $A_y{}^n$, and $A_z{}^n$ by tensor products.[1]

The differential form of the Boltzmann equation is written

$$\partial f_i/\partial t + (A^n f)_i = J(f_i, f_i), \qquad f \in B^n \tag{1}$$

where the nonlinear collision term J is a bilinear form: $B^n \times B^n \to B^n$, which is bounded in the case of cutoff Maxwell molecules. We can write J as a difference

$$J(\varphi, \varphi) = G(\varphi, \varphi) - D(\varphi)\varphi \tag{2}$$

where $G: L_1(\mathbb{R}^3) \times L_1(\mathbb{R}^3) \to L_1(\mathbb{R}^3)$ and $D: L_1(\mathbb{R}^3) \to L_\infty(\mathbb{R}^3)$. For the proofs presented in Section 4 we shall need even more specific assumptions concerning the form of J. In particular, G and D are representable in standard form (and Grad's notation)[2] as integration over a collision kernel:

$$G(\varphi, \varphi)(c) = \int_{S^2}\int_{\mathbb{R}^3} \varphi(c')\varphi(c_1')k(\theta, |c - c_1|)\, dc_1\, d\sigma \tag{3a}$$

$$D(\varphi)(c) = \int_{\mathbb{R}^3} \varphi(c_1) \int_{S^2} k(\theta, |c - c_1|)\, d\sigma\, dc_1 \tag{3b}$$

Here, the two assumptions of cutoff Maxwell molecule force law and angular cutoff combine to assure that $k(\theta, q) \geqslant 0$ is bounded.[2] The proofs of this and the following section are actually valid for any bounded kernel, of which the cutoff Maxwell gas model is an example. In any case, the boundedness restriction will be removed in Section 4.

The collision operator J has the property of conserving mass and energy.[2] In particular, let $(1 + c^2)\varphi \in L_1(\mathbb{R}^3)$. Then from the assumed form of the (bounded) collision operator, one obtains

$$\int_{\mathbb{R}^3} J(\varphi, \varphi)\, dc = 0 \tag{4a}$$

$$\int_{\mathbb{R}^3} c^2 J(\varphi, \varphi)\, dc = 0 \tag{4b}$$

and for positive φ (subject additionally to some technical restrictions).[7]

$$\int_{\mathbb{R}^3} J(\varphi, \varphi) \ln \varphi\, dc \leqslant 0 \tag{5}$$

(This inequality implies an H theorem for the Boltzmann equation.)

In Refs. 1 and 3, it is shown that in order to obtain solutions of Eq. (1), it is equivalent to consider the integral version of Eq. (1):

$$f(t) = U^n(t)\varphi_0 + \int_0^t U^n(t - s)J(f(s), f(s))\, ds \tag{6}$$

where $\varphi_0 \in B^n$ represents the initial datum and $U^n(t)$ is the semigroup generated by A^n. The first two lemmas state properties of the semigroup U^n. Lemma 1 was proved in Ref. 1.

Lemma 1. (a) $U^n(t)B_+{}^n \subset B_+{}^n$.

(b) $U^n(t)$ is a (strongly continuous) contraction semigroup and continues analytically to a bounded holomorphic semigroup.

(c) $\sum_{i\in\Gamma_n} (U^n(t)f)_i = \sum_{i\in\Gamma_n} f_i$ for all $f \in B^n$.

Lemma 1(c) implies immediately particle and energy conservation for the collision-free Boltzmann equation. Indeed, for any $\kappa \geqslant 0$ and $\varphi_0 \in B_\kappa{}^n$,

$$\sum_{i\in\Gamma_n} \int_{\mathbb{R}^3} (1 + c^2)^{\kappa/2} (U^n(t)\varphi_0)_i(c)\, dc = \sum_{i\in\Gamma_n} \int_{\mathbb{R}^3} (1 + c^2)^{\kappa/2} \varphi_{0i}(c)\, dc \qquad (7)$$

Lemma 2. $U^n(t)$ is a contraction semigroup on $B_\kappa{}^n$.

Proof. From Lemma (1a) and Eq. (7), we observe

$$\|U^n(t)f\|_\kappa \leqslant \|f\|_\kappa$$

so $U^n(t)$ is contractive on $B_\kappa{}^n$. For strong continuity, we note that the set

$$\hat{B}^n = \{f \in B^n | f \text{ has compact support}\}$$

is dense in $B_\kappa{}^n$ for all κ, and $U^n(t)$ is strongly continuous on $\hat{B}^n$ by Lemma 1(b). Thus $U^n(t)$ is strongly continuous on $B_\kappa{}^n$, proving the lemma.

We now show particle and energy conservation for the full Boltzmann equation (i.e., with collisions).

Lemma 3. (a) Let $\varphi_0 \in B_+{}^n$ and let $f(t)$ be the solution of Eq. (6) with $f(0) = \varphi_0$. Then $f(t) \in B_+{}^n$ and

$$\|f(t)\|_{B^n} = \|\varphi_0\|_{B^n}$$

(b) Let $\varphi_0 \in B^n_{2,+}$ and $f(t)$ as above. Then

$$\|f(t)\|_2 = \|\varphi_0\|_2$$

Proof. Part (a) is proved in Ref. 1 under the assumption $\varphi_0 \in B_+{}^n \cap D(A)$. [The restriction to $D(A)$ is removed in Ref. 7.] The idea is to integrate Eq. (6) over c and use Eq. (4a).

(b) We mimic the proofs of Ref. 1 for the space $B_2{}^n$ to conclude that for $\varphi_0 \in B^n_{2,+}$ there exists a (unique) solution $f(t) \in B^n_{2,+}$. Then multiplication of Eq. (6) by c^2 and integration, noting Eq. (4b), yields the desired result.

We now consider entropy production, first for the collisionless equation.

Lemma 4. Let $\varphi_0 \in B_+{}^n$, $\varphi_0 \ln \varphi_0 \in B^n$, and define

$$H(\varphi) = \sum_{i\in\Gamma_n} \int_{\mathbb{R}^3} dc\ \varphi_i(c) \ln \varphi_i(c)$$

Then $H(U^n(t)\varphi_0)$ is a nonincreasing function of t.

Proof. The proof of Theorem 1 in Ref. 1 shows that $U^n(t, c)_{ij} \geqslant 0$, where U^n_{ij} indicates the matrix elements

$$(U^n(t)f)_i(c) = \sum_{j\in\Gamma_n} U^n(t, c)_{ij} f_j(c)$$

Since

$$\sum_{i\in\Gamma_n} U^n(t, c)_{ij} = 1$$

by Lemma 1(c), then considering the lattice points as state space and fixing the velocity c, we see that the matrix $U^n(t, c)$ is the transition matrix for a discrete Markov system. Since any space-independent distribution $\psi(t) \in B^n$ is a fixed point of $U^n(t, c)$, standard arguments[9] prove that $H(U^n(t)\varphi_0)$ is nonincreasing. In particular, writing $\alpha(x) = x \ln x$, and utilizing the convexity of α, we obtain

$$\begin{aligned}\sum_{i\in\Gamma_n} \int_{\mathbb{R}^3} dc\ \alpha((U^n(t)\varphi_0)_i) &\leqslant \sum_{i,j\in\Gamma_n} \int_{\mathbb{R}^3} dc\ U^n(t, c)_{ij} \alpha(\varphi_{0j}) \\ &= \sum_{j\in\Gamma_n} \int_{\mathbb{R}^3} dc\ \alpha(\varphi_{0j})\end{aligned}$$

Lemma 5. Let $\varphi_0 \in B^n_{2,+}$ such that $\varphi_0 \ln \varphi_0 \in B^n$. Let $f(t)$ be a solution of Eq. (6) with $f(0) = \varphi_0$. Then $f(t) \ln f(t) \in B^n$, $t \geqslant 0$, and $H(f(t))$ is a nonincreasing function of t.

The proof of this lemma follows from a theorem proved in Ref. 8 (we reduce the more general statement of Ref. 8 to the case needed here):

Let the strongly continuous semigroup $(U(t), t \geqslant 0)$ on B^n satisfy the following properties:

- (U1) $U(t)\varphi \geqslant 0$ for all $\varphi \in B_+{}^n$, $t \geqslant 0$, $\|U(t)\| \leqslant 1$, $t \geqslant 0$.
- (U2) The restriction of $(U(t); t \geqslant 0)$ to $B_2{}^n$ is a strongly continuous semigroup of contractions on $B_2{}^n$.
- (U3) There are M_∞, m_∞ such that $\|U(t)\varphi\|_\infty \leqslant M_\infty e^{m_\infty t}\|\varphi\|_\infty$, $t \geqslant 0$, for all bounded $\varphi \in B_+{}^n$.
- (U4) There are M_0, m_0 such that, for $g(c) = \exp(-1 - c^2)$, $U(t)g \geqslant M_0(\exp m_0 t)g$.
- (U5) If $\varphi \in B^n_{2,+}$ is such that $\varphi \ln \varphi \in B^n$, then $U(t)\varphi \ln U(t)\varphi \in B^n$ for all $t \geqslant 0$, and $H(U(t)\varphi)$ is a nonincreasing function of t.

Let furthermore J be as defined by Eqs. (2) and (3). Then the conclusion of Lemma 5 is true.

Proof of Lemma 5

Properties (U1), (U2), and (U5) are true by Lemmas 1, 2, and 4, respectively. Properties (U3) and (U4) follow immediately from Lemma 1(c), with $M_\infty = 2^{3n}$, $m_\infty = 0$, $M_0 = 1$, $m_0 = 0$. The conditions imposed on J in the general theorem of Ref. 8 can be seen to hold automatically for J defined in Eqs. (2) and (3).

3. WEAK COMPACTNESS AND LATTICE LIMIT

We define the Banach spaces $B = L_1(\Gamma \times \mathbb{R}^3)$ and

$$B_T = L_1([0, T] \times \Gamma \times \mathbb{R}^3)$$

where $\Gamma = [0, 1]^3$. The spaces B_κ and $B_{T,\kappa}$ are then defined in the obvious way (see Section 2). We next introduce the projection $P^n: B \to B^n$ by

$$(P^n(f))_i(c) = 2^{3n} \int_{\Delta_i} f(x, c)\, dx \tag{8a}$$

where Δ_i is a cubical plaquette of side 2^{-n} associated with the ith lattice point. We also define the injections $I^n: B^n \to B$

$$(I^n f)(x, c) = f_i(c), \qquad x \in \Delta_i \tag{8b}$$

When needed for clarity, we may use a superscript n to designate an element of B^n; thus $f^n \in B^n$.

We now obtain uniform bounds on the entropy and energy (with respect to n).

Lemma 6. Let $\varphi_0 \in B_{2,+}$ such that $\varphi_0 \ln \varphi_0 \in B$. Let $f^n(t)$ be the solution of Eq. (6) with $f^n(0) = P^n\varphi_0$. Then $H(f^n(t)) \leqslant H(\varphi_0)$ and

$$\|f^n(t)\|_{B_2^n} = \|\varphi_0\|_{B_2}, \qquad t \geqslant 0$$

Proof. By virtue of the previous lemma, it is sufficient to verify the estimate

$$2^{-3n} \sum_{i \in \Gamma_n} \int_{\mathbb{R}^3} dc\, \alpha((P^n\varphi_0)_i) \leqslant \int dx \int dc\, \alpha(\varphi_0) \tag{9}$$

with $\alpha(x) = x \ln x$. Since $2^{3n} \int_{\Delta_i} dx = 1$, Jensen's inequality[10] and the convexity of α give

$$\alpha\left(2^{3n} \int_{\Delta_i} \varphi_0(x, c)\, dx\right) \leqslant 2^{3n} \int_{\Delta_i} \alpha(\varphi_0(x, c))\, dx$$

Thus the left hand side of (9) is bounded by

$$2^{-3n} \sum_{i\in\Gamma_n} \int_{\mathbb{R}^3} dc\, 2^{3n} \int_{\Delta_i} \alpha(\varphi_0(x, c))\, dx = \int_\Gamma dx \int_{\mathbb{R}^3} dc\, \alpha(\varphi_0)$$

The equality for $\|f^n(t)\|_{B_2^n}$ is immediate.

We are now prepared to state the main result of this section.

Theorem 1. Let $f^n(t)$ be the solution of Eq. (1) with $f^n(0) = P^n\varphi_0$, $\varphi_0 \in B_{2,+}$ and $\varphi_0 \ln \varphi_0 \in B$. Then the sequence $\{I^n f^n\}$ contains a subsequence $\{I^{n_j} f^{n_j}\}$ which converges weakly in B_T for every $T \geqslant 0$.

The theorem is proved by the bounds in Lemma 6 and the following criterion for compactness in L_1 (see Ref. 6). A sequence $\{f^n\}$ of nonnegative functions satisfying the uniform bounds

$$\int_0^T dt \int_{\mathbb{R}^3} dc \int_\Gamma dx\, (1 + c^2) f^n(t, x, c) \leqslant K$$

$$\int_0^T dt \int_{\mathbb{R}^3} dc \int_\Gamma dx\, f^n(t, x, c) \ln f^n(t, x, c) \leqslant K$$

is weakly compact.

We note that, as a consequence of weak convergence, the weak limit f of the subsequence $\{I^{n_j} f^{n_j}\}$ has the property of conservation of mass in the following sense: for any $\chi \in L_\infty(0, T)$ with $\int_0^T \chi(t)\, dt = 1$, we have

$$\|\varphi_0\| = \int f(t, x, c)\, dc\, dx\, \chi(t)\, dt$$

4. BOLTZMANN EQUATION FOR THE NON-MAXWELL GAS

In his treatment of the spatially homogeneous Boltzmann equation, Arkeryd[6] has used compactness arguments to prove the existence of solutions for generalized collision models, i.e., non-Maxwell molecules. We follow Arkeryd's method here to derive similar results for the lattice model.

Assume the collision kernel, as defined in Eqs. (3), obeys the condition

$$0 \leqslant k(\theta, q) \leqslant M(1 + q^\lambda) \tag{10}$$

for some $0 \leqslant \lambda < 2$ and $M > 0$. We define a sequence $\{k_p\}$ of bounded kernels by

$$k_p(\theta, q) = \inf\{k(\theta, q), p\}$$

and write J_p for the collision operator J with kernel k_p. [We observe that for every finite integer p, k_p obeys the conditions stated on J, which guarantee the existence of a global solution to the Boltzmann equation on the lattice as proved in Ref. 1.] We now state the following result:

Theorem 2. Let $\varphi_0 \in B^n_{2,+}$, $\varphi_0 \ln \varphi_0 \in B^n$, and f_p the solution of Eq. (6), with collision kernel k_p, satisfying $f_p(0) = \varphi_0$. Then $\{f_p(t)\}_{p=1}^{\infty}$ contains a subsequence which converges weakly in $B_\kappa{}^n$, $\kappa < 2$. The limit $f(t)$ is continuous, satisfies the bounds $\|f(t)\| = \|\varphi_0\|$, $\|f(t)\|_2 \leqslant \|\varphi_0\|_2$, and obeys Eq. (6) with (unbounded) collision kernel $k(\theta, q)$.

Proof. The compactness criterion stated at the end of the previous section, along with the estimates $H(f_p(t)) \leqslant H(f_p(0)) = H(\varphi_0)$ (Lemma 5) and $\|f_p(t)\|_2 = \|f_p(0)\|_2 = \|\varphi_0\|_2$ (Lemma 3), proves the existence of a subsequence converging weakly in B^n to a function $f(t)$ for a denumerable dense set of t. Extension to all t will follow from the equicontinuity of the family $\{f_p\}_{p=1}^{\infty}$. Also, we note that weak convergence in B^n together with boundedness in $B_2{}^n$ implies weak convergence in $B_\kappa{}^n$ for $\kappa < 2$. To prove equicontinuity we use the fact that f_p is also a solution of Eq. (1).[1,7] Then

$$\|f_p'(t)\| \leqslant \|A^n f_p(t)\| + \|J_p(f_p(t), f_p(t))\|$$

Both terms on the right side have bounds independent of p. For,

$$\|J_p(f_p, f_p)\| \leqslant K(\|f_p\|_2)^2 = K(\|\varphi_0\|_2)^2$$

where K depends only on the bound M in (10). Further, since

$$\|A^n \varphi\| \leqslant 6\|(|c|\varphi)\| \leqslant 6\|\varphi\|_2$$

we have

$$\|A^n f_p(t)\| \leqslant 6\|\varphi_0\|_2$$

Thus $\|f_p(t)\|$ is uniformly bounded in p. Equicontinuity of the sequence $\{f_p\}_{p=1}^{\infty}$ follows.

Conservation of mass, $\|f(t)\| = \|\varphi_0\|$, follows immediately from weak convergence. The energy estimate is a simple application of Fatou's Lemma. We note that $t \to f(t) \in B_\kappa{}^n$ is continuous for $\kappa < 2$. As a result of the bound (10) on the collision kernel, $J\colon B_\lambda{}^n \times B_\lambda{}^n \to B^n$ is continuous, and therefore so is $t \to J(f(t)) \in B^n$.

Since $B_\kappa{}^n$ satisfies the Dunford–Pettis property, $J\colon B_\lambda{}^n \times B_\lambda{}^n \to B^n$ is weakly continuous.[11] In particular, $J(f_p(s))$ converges weakly to $J(f(s))$ for each s. Since $\|J_p(\psi) - J(\psi)\| \to 0$ uniformly for ψ in the unit ball of $B_2{}^n$, we have $J_p(f_p(s)) \xrightarrow{\text{wk}} J(f(s))$ pointwise in s.

Using the integral equation for $f_p(t)$, the Dominated Convergence Theorem, and the established continuity of $J(f(t))$, we can see that the limit function $f(t)$ satisfies Eq. (6).

Theorem 3. In addition to the hypotheses of Theorem 2, let $\varphi_0 \in B_\kappa^n$ for some $\kappa > 2, 2\lambda$. Then $\|f(t)\|_2 = \|\varphi_0\|_2$ (energy conservation).

Proof. The proof is an application of Povzner's inequality[6]:

$$\int_{\mathbb{R}^3} dc\,(1 + c^2)^{\kappa/2} J(\psi, \psi)(c) \leqslant M_\kappa\{\|\,|\psi|\,\|_{\kappa+\lambda-\theta}\|\,|\psi|\,\|_\theta + \|\,|\psi|\,\|_{\kappa-\theta}\|\,|\psi|\,\|_{\lambda+\theta}\}$$

where M_κ is a constant depending only on κ; $0 \leqslant \theta \leqslant 2$; λ is the growth rate of the collision kernel indicated in (10); and the norms $\|\,|\cdot|\,\|_\alpha$ indicate that the spatial variable has not been summed. We may assume, without loss of generality, that $\lambda > 1$. For the choice $\kappa = 2\lambda$, and $\theta = \lambda$, Povzner's inequality and Lemma 2 give

$$\|f_p(t)\|_\kappa \leqslant \|\varphi_0\|_\kappa + M_\kappa^{(n)} \int_0^t \|f_p(s)\|_2 \|f_p(s)\|_\kappa\, ds$$

where $M_\kappa^{(n)}$ is a constant depending both on κ and the lattice spacing. By the Gronwall inequality $\|f_p(t)\|_\kappa$ is uniformly bounded on finite time intervals, and thus the weak subsequence convergence $f_p \to f$ in B^n extends to weak subsequence convergence $f_p \to f$ in $B_{\kappa'}^n$, for any $\kappa' < \kappa$, in particular $\kappa' = 2$. Energy conservation is immediate.

We remark that from the uniformity in p of the bound $H(f_p) \leqslant H(\varphi_0)$ and the energy bound, $\|f(t)\|_2 \leqslant \|\varphi_0\|_2$, the double limit as $p \to \infty$ and the lattice spacing $2^{-n} \to 0$ may be treated to obtain a weakly convergent subsequence for unbounded collision kernels. As we noted, what equation such a limiting solution might obey is not known.

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