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# Transport Properties of the Lorentz Gas: Fourier's Law

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We investigate the stationary nonequilibrium (heat transporting) states of the Lorentz gas. This is a gas of classical point particles moving in a region $\Lambda$ containing also fixed (hard sphere) scatterers of radius $R$. The stationary state considered is obtained by imposing stochastic boundary conditions at the top and bottom of $\Lambda$, i.e., a particle hitting one of these walls comes off with a velocity distribution corresponding to temperatures $T_1$ and $T_2$ respectively, $T_1 < T_2$. Letting $\rho$ be the average density of the randomly distributed scatterers we show that in the Boltzmann–Grad limit, $\rho \to \infty$, $R \to 0$ with the mean free path fixed, the stationary distribution of the Lorentz gas converges in the $L^1$-norm to the stationary distribution of the corresponding linear Boltzmann equation with the same boundary conditions. In particular, the steady state heat flow in the Lorentz gas converges to that of the linear Boltzmann equation, which is known to behave as $(T_2 - T_1)/L$ for large $L$, where $L$ is the distance from the bottom to the top wall: i.e., Fourier's law of heat conduction is valid in the limit. The heat flow converges even in probability. Generalizations of our result for scatterers with a smooth potential as well as the related diffusion problem are discussed.

**KEY WORDS:** Thermal conductivity; low-density (Boltzmann–Grad) limit; kinetic definition of transport coefficients.

## 1. INTRODUCTION

Equilibrium statistical mechanics has various model systems which (a) have a basic structure qualitatively similar to some real systems and (b) exhibit in a precise mathematical form interesting phenomena observed in real systems.

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There is then little doubt that the phenomena of interest in the real system are of the same origin as in the model. We have in mind here particularly the model system for real ferromagnetism, spins on a lattice, for which the existence of a spontaneous magnetization at low temperatures can be proven rigorously.[(1),5] In contrast there are at present no model dynamical systems for which kinetic laws, such as Fourier's law of heat conduction, can be proven to hold. It is the purpose of this note to provide what we believe comes closest to such a model system. (This will also show how far we still are from a real microscopic understanding of nonequilibrium phenomena.)

The system we consider is that of particles moving independently among fixed, "randomly distributed" scatterers. This system is commonly known in statistical mechanics, at least when the scatters are hard spheres—the case we shall primarily consider—as the Lorentz gas[(3),6] or Sinai's billiards.[(5)] It models the scattering of electrons by impurities in a solid. (It is closely related to the simpler Enrenfest wind-tree model,[(6)] where the scatterers are polygons enabling a restriction to a discrete momentum space.) For simplicity the system is confined to a rectangular box $\Lambda \subset \mathbb{R}^3$ with a base and ceiling at $z = 0$ and $z = L$ and a cross-sectional area $B$ in the $x$–$y$ planes. (The analysis will hold for more general $\Lambda \subset \mathbb{R}^d$, $d \geqslant 2$.) Inside the box there are spheres (trees) of radius $R$ located at "random" positions with a density $\rho$. The space outside the spheres is occupied by point (wind) particles of unit mass and density $n$. These particles move freely and are scattered elastically by the fixed spheres.

To induce a heat flow in this system we imagine the bottom and top walls to be kept "cold" and "hot" at temperatures $T_1$ and $T_2$, respectively, $T_1 < T_2$. This means (in the simplest case) the following: a wind particle hitting either the bottom or the top wall will, independent of its incoming velocity, leave the wall with a velocity distribution characteristic of a particle coming from a thermal reservoir at the temperature of that wall.[(7–9)] (We may imagine our particle to interact very strongly with the wall atoms, taking on their temperature almost instantaneously.) At all other walls a wind particle is specularly reflected. (Alternatively, we could use periodic boundary conditions in the $x$ and $y$ directions.)

We ask now for the amount of energy transported per unit time and per unit area $J$ from the hot wall to the cold wall in the steady state, i.e., when the velocity and the spatial distribution of the wind particles, moving under the combination of the deterministic dynamics in the box and the stochastic boundary conditions described above, is stationary. According to Fourier's law we should have for $L \gg (\rho R^2)^{-1}$, which is of the order of the mean free

[5] See Ref. 2 for recent results.

[6] See Ref. 4 for a review of theoretical and experimental work.

path, $J = \kappa(T_2 - T_1)/L$, with $0 < \kappa < \infty$ the thermal conductivity. It is the proportionality between $J$ and $L^{-1}$ for large $L$ that is here the crux of the kinetic law and begs for a derivation in a mathematically convincing way.[10,11]

A little thought shows that in this system the steady-state heat flux is approximately proportional to the fraction of particles, starting on the wall $\{z = 0\}$ with the appropriate velocity distribution, that reach the wall at $\{z = L\}$ before hitting the wall $\{z = 0\}$ again. The proof of the validity of Fourier's law then boils down to showing that this fraction goes asymptotically as $1/L$. Now it is clear that there will be configurations $Q = (Q_1, \ldots, Q_j)$ of scatterers ($Q_i \in \Lambda$ denotes the center of the $i$th scatterer) for which the heat flow $J^Q(L, B)$ will not have the proper asymptotic behavior. Thus, if all the scatterers are located in a box $\Lambda' \subset \Lambda$ bounded by $\{z = 0\}$ and $\{z = L\}$ but only occupying a fraction of the base $B$, then the fraction of particles reaching $\{z = L\}$ will not vanish and $LJ^Q(L, B)$ will diverge as $L \to \infty$. This is what happens in a Knudsen gas[3] or a perfect harmonic crystal,[10–12],[7] but this is clearly the kind of pathology in which we are not interested here. We want to model real systems in which the scatterers (impurities) are "uniformly" distributed throughout the macroscopic region $\Lambda$. We shall translate the above physical statement into appropriate mathematical language as follows: Consider randomly located scatterers whose distribution $\mu^{(R)}$, which may be defined (once and for all) for all of $\mathbb{R}^3$ even though only the part inside $\Lambda$ is relevant, is translation invariant and has "good" cluster properties, i.e., the correlation between the position of scatterers located in different regions decays to zero as the distance between these regions grows to infinity. We then wish to show that the average thermal conductivity $\int d\mu^{(R)}(Q) LJ^Q(L, B)/(T_2 - T_1)$ (computed in the stationary state of the wind particles) approaches a well-defined limit as first $B$ and then $L \to \infty$. Furthermore, in the limit the random variable $LJ^Q(L, B)$ should not fluctuate, i.e., we expect to obtain the same thermal conductivity for almost all configurations.

The averaging over scatterer configurations may be given a direct physical meaning by imagining that the box $\Lambda$ is divided up in boxes $\Lambda_i$ of height $L$ and cross-sectional areas $B_i$, $B = \bigcup_i B_i$. For $B_i$ "sufficiently large" the distribution of scatterers in $\Lambda_i$ as well as the flux through a cross section of $\Lambda_i$ will be approximately independent of what happens in $\Lambda_j$, $j \neq i$. The total flux $J$ will then be an average over the different $J_i$ and will correspond in appropriate limits to the average of $J^Q(L, B)$ over different configurations of scatterers. (This is similar to averaging the free energy in "quenched" systems.)

[7] See Refs. 13 for a harmonic chain with random masses $J_L = cL^{-1/2}$.

Unfortunately we cannot prove the pseudotheorem outlined above even for the simplest case where the distribution of the scatterers is a simple Poisson process with density $\rho$. The difficulty lies in the fact that the motion of the wind particle through $\Lambda$, now considered as a stochastic process where the various paths are weighted according to the probability of the corresponding configuration of scatterers, is *not* a Markov process. The wind particle remembers the scatterer with which it has previously collided. This is what distinguishes this dynamical system from ones described by a linear Boltzmann equation in which the process is Markovian: The particle is scattered in a certain direction with a certain probability depending on the differential cross section *independent* of its past history, where Fourier's law can be readily proven.[14] It is known, however, that in the Boltzmann–Grad limit [corresponding to the density of scatterers $\rho \to \infty$, their radius $R \to 0$ in such a way that the mean free path $(\rho R^2)^{-1}$ is kept constant, while the fraction of volume $\rho R^3$ occupied by the scatterers vanishes], the motion of the wind particles is indeed described by a linear Boltzmann equation.[15–17] The reason for this transition to a Markovian behavior is that in this limit the probability of a wind particle colliding more than once with the same scatterer during any *fixed* time interval $\tau$ vanishes. Using this fact, we shall establish the following results:

(i) The steady state $f^{(R)}(q, p)$ of the Lorentz gas (with the above-mentioned stochastic boundary conditions) converges almost everywhere to the steady state of the linear Boltzmann equation (with the same boundary conditions) in the Boltzmann–Grad limit $R \to 0$.

(ii) Let $J^Q(q; L)$ be the steady-state heat flux at the point $q$ (through a cross-sectional area parallel to the $x$–$y$ plane) for a given configuration $Q$ of scatterers with radius $R$ and let $J^{(R)}(q; L)$ be $J^Q(q; L)$ averaged over the Poisson distribution of scatterers with density $R^{-2}\rho$. Let $J(q; L)$ be the steady-state heat flux at point $q$ obtained from the steady state of the linear Boltzmann equation with collision rate $\rho$, which for $L \ll \rho^{-1}$ is proportional to $(T_2 - T_1)/L$. Then given any $\epsilon > 0$ we can find an $R$ sufficiently small such that $|J^{(R)}(q; L) - J(q; L)| < \epsilon/L$, i.e., for fixed $L$ the difference in the thermal conductivities can be made arbitrarily small.

(iii) The random heat flux $Q \to J^Q(q; L)$ converges in probability to $J(q; L)$ in the Boltzmann–Grad limit $R \to 0$. (The same result holds for all averages in the steady state.)

In Section 2 we study the stationary state of the Lorentz gas. In Section 3 we briefly describe what is known about the stationary solution of the linear Boltzmann equation subject to the stochastic boundary conditions described above. In Section 4 we prove the convergence of the stationary distributions. In Section 5 we comment upon generalizations of our model, in particular to the case of scatterers with a smooth potential.

## 2. THE STATIONARY STATE OF THE LORENTZ GAS

We choose a box $\Lambda \subset \mathbb{R}^3$ with volume $|\Lambda|$ orientated along the coordinate axis with bottom at $\{z = 0\}$ and top at $\{z = L\}$. Inside the box we have randomly distributed hard sphere scatterers. The phase space of the scatterers is $\Gamma = \bigcup_{j \geq 0} \Lambda^j$. We let $Q \in \Gamma$ stand for a configuration of scatterers of radius $R$. Since the scatterers are indistinguishable, their distribution is specified by a probability measure on all finite subsets of $\Lambda$, which in the usual way can be thought of as a symmetric measure $\mu^{(R)}$ on $\Gamma$. We assume that $\mu^{(R)}$ is the Poisson distribution with densities

$$\left\{\frac{1}{j!}\exp[-|\Lambda|(\pi R^2)^{-1}\rho](\pi R^2)^{-j}\rho^j\right\}_{j \geqslant 0} \tag{1}$$

The reason for setting the density equal to $\rho/\pi R^2$ is related to taking the Boltzmann–Grad limit, as will become clear later. Note that we are permitting the scatterers to overlap. But our results also hold for nonoverlapping scatterers.

The Lorentz gas is an ideal gas moving among the scatterers. Since there is no interaction between the gas particles, we can reduce the problem to the motion of a single particle. Let $(q, p) = (x, y, z, p) \in \Lambda \times \mathbb{R}^3$ denote the position and momentum of the moving particle. For a fixed configuration of scatterers $Q$, let $(q, p) \mapsto T_t^Q(q, p)$ be the mechanical motion defined by free motion and *specular* reflection upon hitting either one of the scatterers or the boundary of $\Lambda$. On the phase space where incoming and reflected momentum are identified $T_t^Q$ is a smooth flow which preserves the Lebesgue measure. For the flow to be defined for (almost) all initial conditions $(q, p) \in \Lambda \times \mathbb{R}^3$ we assume that $T_t^Q(q, p) = (q, p)$ if $|q - Q_i| < R$ for some $Q_i$, where $Q = (Q_1, ..., Q_j)$, i.e., a particle inside a scatterer just stays there.

We want the surface $\{z = 0\}$ to model a "cold" reservoir and the surface $\{z = L\}$ a "hot" reservoir. We do this by assuming a stochastic gas–surface interaction.[8,9] One can easily imagine more sophisticated, even mechanical versions of a heat reservoir. But, after all, the thermal conductivity should be a property of the system and insensitive to the detailed nature of the heat reservoir. A natural choice for the stochastic boundary condition would be that the moving particle arriving at the bottom (top) wall is emitted with a Maxwellian velocity distribution corresponding to the temperature of that wall. However, the structure of the steady state is more clearly displayed without such specific assumptions. Let us introduce polar coordinates $(\Omega, v) = (\phi, \theta, v)$ for the momentum $p$ and let $e$ be the inward normal at the surface of $\Lambda$. If the particle arrives at the $\alpha$th wall ($\alpha = 1$ stands for the bottom wall and $\alpha = 2$ stands for the top wall), then, independent of its incoming velocity, its outgoing velocity at the same point will be in $p + dp$ with probability $\max(0, e\cdot p)\, \rho_\alpha(p)\, dp$. Now $\rho_\alpha$, $\alpha = 1, 2$, is assumed to depend only on the speed, $\rho_\alpha(p) = \rho_\alpha(|p|)$, and by definition has to be normalized to

$$\pi \int_0^\infty dv\, v^3 \rho_\alpha(v) = 1 \tag{2}$$

We assume that the first three moments of $\rho_\alpha$ are finite. The emission probability is chosen in such a way that for $\rho_1 = \rho_2 = \rho$, $\rho(p)dp \times$ (uniform distribution outside the scatterers) is stationary. (More general stochastic boundary conditions will be discussed in Section 5.)

At this point it is convenient to change to the language of stochastic processes. Let $\Delta$ be the set of all possible trajectories $(q(t), p(t)) = X(t)$. The $q(t)$ takes values in $\Lambda$, $p(t)$ in $\mathbb{R}^3$. The set $\Delta$ consists of all paths that are piecewise of the form of free motion, i.e., of the form $t \mapsto (q + pt, p)$. A probability measure on $\Delta$ defines then in the usual way a stochastic process. In our model we have to distinguish three different types of processes. For a fixed configuration $Q$ of scatterers we have the process given by the mechanical evolution $T_t^Q$ and the stochastic transition at $\{z = 0\}$ and $\{z = L\}$ as described above. Starting the particle at $(q, p)$, this defines a Markov process on $\Delta$ with measure $P^Q(\cdot\,|q, p)$. Averaging over the scatterers defines a new process on $\Delta$ with measure

$$P^{(R)}(\cdot\,|q, p) = \int_\Gamma d\mu^{(R)}(Q)\, P^Q(\cdot\,|q, p) \tag{3}$$

This process describes the evolution of the Lorentz gas. The crucial point, which makes for all the difficulty in the problem, is that this process is non-Markovian. If the Lorentz particle collides with one of the scatterers twice, then, because of the mechanical evolution, these two scattering events are dependent. In fact, it is the non-Markovian nature of this process that is responsible for such interesting physical effects as the long-time tail of the velocity autocorrelation function.[18] Finally, as $R \to 0$, we obtain a process $X(t)$ on $\Delta$ with measure $P(\cdot\,|q, p)$ which is again Markovian (but nonmechanical). Its transition probability is determined by a linear Boltzmann equation. This process will be described in more detail in the next section.

A word on our notation: A quantity that depends on the specific configuration $Q$ of scatterers is denoted by a superscript $Q$—e.g., $J^Q(q; L)$ is the heat flow for the fixed configuration $Q$ at the point $q$. Its average over the Poisson distribution (1) is denoted by a superscript $(R)$—e.g., the average heat flux is $J^{(R)}(q; L)$. Here we indicate explicitly the $R$ dependence, since we want to investigate the limit $R \to 0$. Finally, the corresponding quantities obtained from the linear Boltzmann equation have no superscript—e.g., $J(q; L)$ is the heat flow at the point $q$ as given by the linear Boltzmann equation.

We turn to the problem of finding a convenient expression for the stationary state of the Lorentz gas. It turns out that the stationary state can be expressed in terms of absorption probabilities, which therefore will be defined now. In addition, the absorption probabilities are the natural objects for which the existence of the Boltzmann–Grad limit can be proved.

Let $\partial\Lambda = \{z = 0\} \cup \{z = L\} \subset \Lambda$ be the surfaces with temperatures. Let $(q, p)$ be the initial point and let us follow the trajectory $T^Q_{-t}(q, p)$, $t \geqslant 0$, i.e., backward in time, until it first reaches the surface $\partial\Lambda$ at a certain point denoted by $q_0$. We define a probability measure $P^Q_{\text{abs}}(\cdot\,|q, p)$ on $\partial\Lambda$ by the prescription that $P^Q_{\text{abs}}(A|q, p) = 1$ if $q_0 \in A$, and $P^Q_{\text{abs}}(A\{q, p) = 0$ if $q_0 \notin A$ for any measurable set $A \subset \partial\Lambda$. [$P^Q_{\text{abs}}(\cdot\,|q, p)$ is a delta function at $q_0$.] $P^Q_{\text{abs}}(\cdot\,|q, p)$ is also the probability that, for a fixed configuration $Q$, the particle is absorbed in the set $A$, following its trajectory forward in time, given that the particle started at position $q$ with velocity $-p$, i.e., at $(q, -p)$. This latter prescription may be used to define the absorption probabilities $P^{(R)}_{\text{abs}}(A|q, p)$ and $P_{\text{abs}}(A|q, p)$ for the Lorentz process $X(t)$ with measure $P^{(R)}(\cdot\,|q, p)$ and for the Markov process $X(t)$ with measure $P(\cdot\,|q, p)$ corresponding to the linear Boltzmann equation. Clearly, $P^{(R)}_{\text{abs}}(A|q, p) = \int d\mu^{(R)}(Q)\, P^Q_{\text{abs}}(A|q, p)$.

For hard sphere scatterers the absorption probabilities are independent of the initial speed $v$. Because of this simplifying feature and because $\rho_\alpha$ depends only on $v$, only the probability of being absorbed by either the bottom or the top wall enters the analysis. We denote these probabilities by $P_\alpha{}^Q(q, \Omega)$, $P^{(R)}_\alpha(q, \Omega)$, and $P_\alpha(q, \Omega)$, $\alpha = 1, 2$ ($\alpha = 1$ stands for being absorbed at the bottom wall and $\alpha = 2$ stands for being absorbed at the top wall). Now $P_1{}^Q(q, \Omega) = 1$, if $T_t{}^Q(q, -p)$, $t \geqslant 0$, $p/|p| = \Omega$, reaches first the bottom wall, and $P_1{}^Q(q, \Omega) = 0$, if $T_t{}^Q(q, -p)$, $t \geqslant 0$, reaches first the top wall. Again, $P^{(R)}_\alpha(q, \Omega) = \int d\mu^{(R)}(Q)\, P_\alpha{}^Q(q, \Omega)$.

We now want to find the stationary state of the Lorentz gas with the specified boundary conditions. For every fixed configuration $Q$ of scatterers a stationary distribution of the Markov process with measure $P^Q(\cdot\,|q, p)$ has to satisfy the following three conditions:

1. $f^Q$ is constant along the flow lines of $T_t{}^Q$. Here a flow line terminates if it hits either one of the surfaces $\{z = 0\}$ and $\{z = L\}$. We have $f^Q(q, p) = 0$ for $q$ inside a scatterer.

2. The assumed nature of the boundary scattering and the requirement that incoming flux equals outgoing flux at every point of the wall leads to the conditions for $e\cdot p \geqslant 0$

$$\begin{aligned} f^Q(x, y, 0, p) &= \rho_1(p) \int_{\{e\cdot p' \leqslant 0\}} dp'\, |e\cdot p'| f^Q(x, y, 0, p') \\ f^Q(x, y, L, p) &= \rho_2(p) \int_{\{e\cdot p' \leqslant 0\}} dp'\, |e\cdot p'| f^Q(x, y, L, p') \end{aligned} \tag{4}$$

3. Constant density $n$:

$$\int_{\Lambda \times \mathbb{R}^3} dq\, dp\, f^Q(q, p) = n|\Lambda| \tag{5}$$

(We shall take $n = 1$ from now on.)

We claim that

$$f^Q(q, p) = \left[\sum_{\alpha=1}^{2} \rho_\alpha(v) P_\alpha{}^Q(q, \Omega)\right] \Big/ N(Q) \tag{6}$$

where $N(Q)$ (assumed to be different from zero) is defined through

$$\int_{\Lambda \times \mathbb{R}^3} dq\, dp\, f^Q(q, p) = |\Lambda|$$

satisfies the conditions 1–3 and is therefore a stationary distribution.

Clearly, $f^Q$ is constant along the flow lines of $T_t{}^Q$. We check the boundary condition at $\{z = 0\}$. The first equation reduces, since $P_2{}^Q(x, y, 0, \Omega) = 0$ for $e \cdot \Omega \geqslant 0$, to

$$1 = \frac{1}{\pi} \int_{\{e \cdot \Omega \leqslant 0\}} d\Omega\, (-\cos\theta)[P_1{}^Q(x, y, 0, \Omega) + P_2{}^Q(x, y, 0, \Omega)] \tag{7}$$

Equation (7) will be satisfied since $P_1{}^Q(x, y, 0, \Omega) + P_2{}^Q(x, y, 0, \Omega) = 1$, unless the trajectory starting at $(x, y, 0, -\Omega)$ reaches neither $\{z = 0\}$ nor $\{z = L\}$. By the Poincaré recurrence theorem, however, this can be the case only for a set of angles with zero $d\Omega$-measure.

In a natural way the "stationary" distribution $f^{(R)}$ of the Lorentz gas is defined as the average of $f^Q$ over $\mu^{(R)}$. Note that $f^{(R)}$ does not satisfy an invariance condition familiar from the Markovian case. Indeed $f^{(R)}$ will not be stationary under the process $P^{(R)}(\cdot\,|\,q, p)$. Nevertheless, we believe, for reasons given in the introduction, that this is the natural and right definition. As we shall also see later, if we consider the expectation value of some observable $g$ (e.g., the heat flux), $\int dq\, dp\, f^Q(q, p) g(q, p)$, then it will equal its average for most configurations if $R$ is chosen small enough. Therefore we obtain as the stationary distribution $f^{(R)}$ of the Lorentz gas with the specified boundary conditions

$$f^{(R)}(q, p) = [\mu^{(R)}(\Gamma_0)]^{-1} \int_{\Gamma_0} d\mu^{(R)}(Q)\, N(Q)^{-1} \left[\sum_{\alpha=1}^{2} \rho_\alpha(v) P_\alpha{}^Q(q, \Omega)\right] \tag{8}$$

with $\Gamma_0 = \{Q \in \Gamma | N(Q) > 0\}$.

We can now define the steady-state heat flux $J^Q(q; L)$ at the point $q$ through a cross-sectional area parallel to the $x$–$y$ plane for a fixed configuration $Q$ of scatterers by

$$J^Q(q; L) = \tfrac{1}{2} \int dp\, p_z p^2 f^Q(q, p) \tag{9}$$

and the average heat flux by

$$J^{(R)}(q; L) = \tfrac{1}{2} \int dp\, p_z p^2 f^{(R)}(q, p) \tag{10}$$

where $p_z$ is the $z$ component of the momentum $p$. Local density and local temperature are defined in an analogous way.

Note that we did not claim uniqueness of $f^Q$. There is one trivial reason for nonuniqueness. Depending on the configuration $Q$, there may exist a set of nonzero measure of trajectories that never hit the bottom and top wall. On this set we can choose any distribution invariant under the flow $T_t^Q$. However, in the Boltzmann–Grad limit, the probability of the set of such configurations converges to zero. If scatterers are not permitted to overlap, presumably, this will be true for all densities below close-packing. We believe that for configurations of scatterers that leave $\Lambda$ connected, (6) is the unique stationary measure on the set of all trajectories hitting bottom and top wall and is unique among all measures that are absolutely continuous with respect to $dq\, dp$. Furthermore, there are good reasons to believe that (6) is not only unique (i.e., ergodic), but also that every initial distribution on trajectories hitting bottom or top walls converges weakly to $f^Q$ in the limit as $t \to \infty$. If this is true for almost all configurations of scatterers, then the stationary distribution $f^{(R)}$ has a natural interpretation: in the limit of $t \to \infty$ the state of the Lorentz gas approaches weakly $f^{(R)}$ (provided the normalization is chosen correctly).

## 3. THE STATIONARY STATE IN THE BOLTZMANN–GRAD LIMIT

To conclude that Fourier's law is approximately valid for small $R$ we have to show first that it holds in the Boltzmann–Grad limit $R \to 0$, where the motion of the particle is described by a linear Boltzmann equation. We therefore describe in this section the nature of this limit and discuss the stationary state of the resulting linear Boltzmann equation with the stochastic boundary conditions specified in Section 2. The problem of the convergence of stationary states $f^{(R)}$ to the stationary state of the Boltzmann equation is taken up in the next section.

The measures $\mu^{(R)}$ in (1) are written in the form appropriate for the Boltzmann–Grad limit: The mean free path of the moving particle remains constant as $R \to 0$ while the density of scatterers goes to infinity and the mean volume occupied by scatterers goes to zero. In this Boltzmann–Grad limit the probability of a particle colliding more than once with the same scatterer within any fixed time interval goes to zero. This in turn implies that all non-Markovian effects are eliminated in the limit and that the time evolution of the Lorentz gas is then governed by a linear Boltzmann equation.

In fact, one can prove[17] that all the finite-dimensional distributions $P^{(R)}(X(t_1) \in A_1, \ldots, X(t_n) \in A_n | q, p)$ converge as $R \to 0$ to $P(X(t_1) \in A_1, \ldots X(t_n) \in A_n | q, p)$. It turns out that $P(\cdot | q, p)$ is a Markov process sometimes called a random flight process. The particle leaves the point $q$ in direction $\Omega$ with speed $v$. The probability of a first collision (random jump in $\Omega$) in the time interval between $t$ and $t + dt$ is $\rho v e^{-\rho v t} \, dt$. Independent of the time of collision the particle is then scattered in the cone $\Omega' + d\Omega'$ with probability $(1/4\pi) \, d\Omega'$. (In general, the scattering law is more complicated and, in particular, depends on the incoming direction $\Omega$. Isotropic scattering is a peculiarity of hard-sphere scatterers in three dimensions.) The process continues then in the same fashion: the probability of a second collision a time $\tau$ later in the time interval $d\tau$, $\tau > 0$, is $\rho v e^{-\rho v \tau} \, d\tau$, etc. Whenever the first particle hits either the bottom or the top wall it will be scattered with the transition probability defined in Section 2. At all other surfaces the particle is specularly reflected.

The time evolution of a probability density $f$ under this process is given by the linear Boltzmann equation

$$
\begin{aligned}
\frac{\partial}{\partial t} f(q, p, t) &= -p \frac{\partial}{\partial q} f(q, p, t) \\
&\quad + \rho |p| \left[ \frac{1}{4\pi} \int_{S^2} d\Omega' f(q, \Omega', v, t) - f(q, p, t) \right] \\
&= (\mathscr{L} f)(q, p, t) \qquad (11)
\end{aligned}
$$

with collision rate $\rho$ together with the stochastic boundary conditions.

We shall now investigate the stationary solutions of (11). A stationary solution $f$ has to satisfy $\mathscr{L} f = 0$ and conditions 2 and 3 of Section 2. As in Section 2, one checks that these conditions are indeed satisfied for

$$
f(q, p) = N^{-1} \sum_{\alpha=1}^{2} \rho_\alpha(v) P_\alpha(q, \Omega) \qquad (12)
$$

with $N$ determined through

$$
|\Lambda| N = \sum_{\alpha=1}^{2} \int_0^\infty dv \, v^2 \rho_\alpha(v) \int_{\Lambda \times S^2} dq \, d\Omega \, P_\alpha(q, \Omega)
$$

It can be shown that $f$ is the *unique* stationary measure and that any initial measure converges exponentially fast to it as $t \to \infty$.[19] [The condition $\mathscr{L} f = 0$ involves rather delicate domain questions. Avoiding these problems, in Ref. 14 the stationary solution (12) is obtained as a limit $t \to \infty$ starting with a suitable initial distribution.]

To get some idea of what the stationary distribution looks like, we should find the absorption probabilities $P_\alpha(q, \Omega)$. For the Boltzmann equation they cannot be computed explicitly. [Obviously, they are related to the widely studied slab albedo problem,[20,21] where one is basically interested in $P_2(0, \Omega)$.] Using the reults of Ref. 14, which apply to more general cases, we have, however, the following rigorous estimates:

$$\frac{z + \rho^{-1}\cos\theta}{L + \rho^{-1}} \leqslant P_2(q, \Omega) \leqslant \frac{z + \rho^{-1}(1 + \cos\theta)}{L + \rho^{-1}}$$
$$P_1(q, \Omega) + P_2(q, \Omega) = 1 \tag{13}$$

and

$$\frac{4\pi}{3}\frac{1}{\rho L + 2} \leqslant \int_{S^2} d\Omega \cos\theta\, P_2(q, \Omega) \leqslant \frac{4\pi}{3}\frac{1}{\rho L} \tag{14}$$

There is a simple intuitive argument why (13) should be true. If one divides $\Lambda$ into $n$ horizontal slabs of thickness $d$ by planes $S_j$, $j = 1,..., n - 1$, then starting on any $S_l$ the particle should have equal probability of reaching $S_{l-1}$ or $S_{l+1}$. Since hitting the top or bottom requires transversing intervening planes whose number is proportional to $L - z$ and $z$, respectively, their respective probabilities should be in ratio $z/(L - z)$, which leads to $P_2(q, \Omega) = z/L$. The result (13) shows that this argument is indeed correct up to errors of the order of a mean free path.

Using (13) and (14), one can easily compute the local density, the temperature profile, and the heat flow for $L \gg \rho^{-1}$. We give here only the expression for the heat flow in the case where $\rho_1$ and $\rho_2$ are Maxwellians corresponding to temperatures $T_1$ and $T_2$ normalized as in (2). We obtain

$$J(q; L) = \frac{8}{3}\left(\frac{2}{\pi}\right)^{1/2} \frac{(T_1 T_2)^{1/2}}{\sqrt{T_1} + \sqrt{T_2}} \frac{1}{\rho} \frac{T_1 - T_2}{L}, \qquad L \gg \rho^{-1} \tag{15}$$

which is of the form expected from Fourier's law. For $T_1$ and $T_2$ close to $T$ the thermal conductivity behaves as $\rho^{-1}\sqrt{T}$.

It is instructive to rewrite the stationary state (12) using the asymptotic behavior of $P_\alpha(q, \Omega)$. In general, close to equilibrium, one would expect a steady state of the form

$$f = f_0 + (\nabla T) f_1 + \cdots \tag{16}$$

$f_0$ is a state of "local equilibrium" and $(\nabla T) f_1$ gives the correction to local equilibrium which is of the order $1/L$, since $\nabla T \sim 1/L$. By itself $f_1$ should have a well-defined limit as $L \to \infty$ and averages over $f_1$ would yield the transport coefficients, e.g., the thermal conductivity $\chi(q)$ in the infinite-volume limit would be given by $\chi(q) = \frac{1}{2}\int dp\, p_z\, p^2 f_1(q, p; T_1, T_2, L = \infty)$.

As in equilibrium, the infinite-volume limit is taken to avoid boundary corrections.

For a Boltzmann fluid (i.e., one where the one-particle distribution function evolves according to the nonlinear Boltzmann equation), (16) formally results from the Enskog expansion with local equilibrium defined as local Maxwellian corresponding to density, momentum, and energy density. Using (14), we can prove (16) in the case of the linear Boltzmann equation. Since energy is conserved in a collision, local equilibrium does not correspond to local Maxwellian, but rather to a distribution

$$f_0(q,p) = \sum_{\alpha=1}^{2} a_\alpha(q)\rho_\alpha(p) \tag{17}$$

where $a_1(q)$ and $a_2(q)$ are determined such that $f_0(q,p)$ has the same density and energy density as $f(q,p)$. For large $L$, one obtains

$$f_0(q,p) = N^{-1}\left[\rho_1(v)\frac{L-z}{L} + \rho_2(v)\frac{z}{L}\right] \tag{18}$$

and the correction term $(\nabla \cdot T)f_1$ as

$$[(\nabla \cdot T)f_1](q,p;T_1,T_2,L) = N^{-1}[\rho_1(v) - \rho_2(v)]\frac{\cos\theta}{L\rho} \tag{19}$$

It is clear that $\lim_{L\to\infty} f_1(q,p;T_1,T_2,L)$ exists. However, if we move both the bottom and top wall to infinity as $z_{\text{bottom}} = -aL$ and $z_{\text{top}} = L$, $a > 0$, then the limit will depend on $a$. If we consider a small temperature difference

$$\lim_{\varepsilon\to 0}\lim_{L\to\infty} f_1(q,p;T-\epsilon,T+\epsilon,L) \tag{20}$$

then this limit exists and is *independent* of the way we took the infinite-volume limit. In the case where $\rho_1$ and $\rho_2$ are Maxwellians, one obtains

$$\lim_{\varepsilon\to 0}\lim_{L\to\infty} f_1(q,p;T-\epsilon,T+\epsilon,L) = \frac{1}{8\pi}\left(\frac{2}{\pi}\right)^{1/2}\frac{\cos\theta}{\rho T^{7/2}}(-v^2+4T)\exp\left(-\frac{v^2}{2T}\right) \tag{21}$$

We note that the density flux $\int dp\, p f_1(q,p) = 0$.

We expect a corresponding situation for the Lorentz gas with finite $R$. The results of the next section indicate that, at least for small $R$, this expectation is quite reasonable. However, since we cannot control the limit $R \to 0$ uniformly in $L$, there is at the present no proof that $\lim_{L\to\infty} f_1^{(R)}(L)$ exists for the Lorentz gas.

## 4. APPROACH OF STATIONARY STATES TO THE BOLTZMANN–GRAD LIMIT

The convergence of the dynamics of the Lorentz gas as $R \to 0$ to the dynamics described by the linear Boltzmann equation is proved in Ref. 17 for a fixed time $t$. The convergence of stationary states poses the additional difficulty that the absorption time (for those trajectories that are absorbed) is unbounded with a finite expectation. We first prove:

**Lemma 1.** The absorption probabilities converge pointwise

$$\lim_{R \to 0} P_\alpha^{(R)}(q, \Omega) = P_\alpha(q, \Omega), \qquad \alpha = 1, 2 \tag{22}$$

*Proof.* To simplify notation we set $v = 1$ and omit the argument $v$. We consider all paths that reach the top wall before hitting the bottom wall. If the particle collides $n$ times with scatterers before reaching the top wall, we parametrize the path in the following way: The particle starts at $(q, \Omega)$. It travels with unit speed a time $t_1$, including specular reflection at the boundaries with no temperature. This defines the first collision point, provided that the particle did not reach the walls with temperature. The particle is then scattered by an angle $\Omega_1$ relative to the incoming velocity and travels with unit speed a time $t_2$. This defines the second collision point, provided that the particle did not reach the walls with temperature, etc. We require that the $(n + 1)$th collision point is at the top wall. The latter condition fixes $t_{n+1}$. Therefore a path with $n$ collisions is specified by $(t_1, \Omega_1, \ldots, t_n, \Omega_n)$. Let $r_j \in \mathbb{R}^3$ be the vector with polar coordinates $(t_j, \Omega_j)$ and let us denote by $\Gamma_n(q, \Omega) \subset \mathbb{R}^{3n}$ the set of all paths that start at $(q, \Omega)$ and that reach the top wall before hitting the bottom wall with precisely $n$ collisions.

Let $\Gamma_n^{(R)}(q, \Omega) \subset \mathbb{R}^n$ be the set of all paths starting at $(q, \Omega)$ such that after $n$ collisions they reach the top wall before hitting the bottom wall and such that every scatterer collided with is hit precisely once. Then the absorption probability $P_\alpha^{(R)}(q, \Omega)$ can be split into two parts

$$P_\alpha^{(R)}(q, \Omega) = P_{\alpha,s}^{(R)}(q, \Omega) + P_{\alpha,r}^{(R)}(q, \Omega) \tag{23}$$

$P_{\alpha,s}^{(R)}(q, \Omega)$ accounts for all paths in $\Gamma_n^{(R)}(q, \Omega)$ and the remainder $P_{\alpha,r}^{(R)}(q, \Omega)$ contains all multiple scattering events. Let $V^{(R)}(q, \Omega | r_1, \ldots, r_n)$ be the volume of $\{q' \in \Lambda \mid |q - q'| \geqslant R, |q(t) - q'| \leqslant R, q(t)$ moving along the path specified by $r_1, \ldots, r_n\}$. Then

$$P_{2,s}^{(R)}(q, \Omega) = \sum_{n=0}^{\infty} \frac{1}{n!} (\pi R^2)^{-n} \rho^n \int_{\Gamma_{n,s}} dQ_1 \cdots dQ_n \\ \times \exp[-(\pi R^2)^{-1} \rho V^{(R)}(q, \Omega | r_1, \ldots, r_n)] \tag{24}$$

$\Gamma_{n,s}$ is the set of all configurations of $n$ scatterers producing a path in $\Gamma_n^{(R)}(q, \Omega)$, and $V^{(R)}(q, \Omega|r_1,..., r_n)$ is considered here as a function of $Q_1,..., Q_n$. Going over to the coordinates of the path, the volume element transforms as

$$dQ_1 \cdots dQ_n = \left(\frac{R^2}{4}\right)^n \prod_{j=1}^{n} dt_j\, d\Omega_j$$

Taking into account that the $n$! permutations of the $n$ scatterers produce the same path, we obtain

$$P_{2,s}^{(R)}(q, \Omega) = \sum_{n=0}^{\infty} \left(\frac{\rho}{4\pi}\right)^n \int_{\Gamma_n^{(R)}(q,\Omega)} \prod_{j=1}^{n} dt_j\, d\Omega_j \times \exp[-(\pi R^2)^{-1}\rho V^{(R)}(q, \Omega|r_1,..., r_n)] \tag{25}$$

Let $P_{2,s,n}^{(R)}(q, \Omega)$ be the $n$th term in the sum (25). As $R \to 0$, $\Gamma_n^{(R)}(q, \Omega) \to \Gamma_n(q, \Omega)$. For small $R$, $V^{(R)}(q, \Omega|r_1,..., r_n)$ is a small tube around the actual path, implying that $(\pi R^2)^{-1} V^{(R)}(q, \Omega|r_1,..., r_n)$ converges to $t_1 + \cdots + t_{n+1}$. Therefore we expect that

$$\lim_{R\to 0} P_{2,s,n}^{(R)}(q, \Omega) = P_{2,n}(q, \Omega) = \left(\frac{\rho}{4\pi}\right)^n \int_{\Gamma_n(q,\Omega)} \prod_{j=1}^{n} dt_j\, d\Omega_j \exp\left(-\rho \sum_{j=1}^{n+1} t_j\right) \tag{26}$$

We show that the integrand $\exp[-(\pi R^2)^{-1}\rho V^{(R)}(q, \Omega|r_1,..., r_n)]$ has an integrable bound uniform in $R$. Then (26) follows by dominated convergence. By inspection

$$(\pi R^2)^{-1} V^{(R)}(q, \Omega|r_1,..., r_n) \geqslant \frac{1}{n} \sum_{j=1}^{n} |r_j| \tag{27}$$

and therefore

$$\int_{\mathbb{R}^{3n}} \left(\prod_{j=1}^{n} |r_j|^{-2}\, dr_j\right) \exp[-(\pi R^2)^{-1} V^{(R)}(q, \Omega|r_1,..., r_n)] \leqslant \left(\frac{4\pi n}{\rho}\right)^n \tag{28}$$

From the probabilistic interpretation of the linear Boltzmann equation described in Section 3 we conclude that

$$P_2(q, \Omega) = \sum_{n=0}^{\infty} P_{2,n}(q, \Omega) \tag{29}$$

To show that the sum (25) converges to the sum (29) and that the remainders in (23) converge to zero as $R \to 0$ we use positivity and normalization. We have[14]

$$\sum_{\alpha=1}^{2} P_\alpha(q, \Omega) = 1 \tag{30}$$

By (23) and by the Lemma of Fatou

$$1 \geqslant \sum_{\alpha=1}^{2} P_{\alpha,s}^{(R)}(q,\Omega) \geqslant \sum_{\alpha=1}^{2} \liminf P_{\alpha,s}^{(R)}(q,\Omega) \geqslant \sum_{\alpha=1}^{2} P_\alpha(q,\Omega) = 1 \tag{31}$$

Therefore $\liminf P_{\alpha,s}^{(R)}(q,\Omega) = P_\alpha(q,\Omega)$. Furthermore,

$$\begin{aligned}\limsup P_{1,s}^{(R)}(q,\Omega) &\leqslant \limsup \sum_{\alpha=1}^{2} P_{\alpha,s}^{(R)}(q,\Omega) + \limsup[-P_{2,s}^{(R)}(q,\Omega)] \\ &\leqslant 1 - P_2(q,\Omega) = P_1(q,\Omega)\end{aligned} \tag{32}$$

Therefore

$$\lim_{R\to 0} P_{\alpha,s}^{(R)}(q,\Omega) = P_\alpha(q,\Omega) \tag{33}$$

Since

$$1 \geqslant \sum_{\alpha=1}^{2} P_{\alpha}^{(R)}(q,\Omega) = \sum_{\alpha=1}^{2} [P_{\alpha,s}^{(R)}(q,\Omega) + P_{\alpha,r}^{(R)}(q,\Omega)]$$

and by (30) and (33)

$$\lim_{R\to 0} \sum_{\alpha=1}^{2} P_{\alpha,r}^{(R)}(q,\Omega) = 0 \tag{34}$$

Since $\sum_{\alpha=1}^{2} P_{\alpha,r}^{(R)}(q,\Omega) \geqslant 0$, (34) together with (33) proves (22). ∎

If we consider $P_\alpha{}^Q(q,\Omega)$ as random variables on $\Gamma$ with measure $\mu^{(R)}$, then it is easy to convince oneself that their variance converges to $P_1(q,\Omega) \times P_2(q,\Omega)$ in the Boltzmann–Grad limit and they therefore still fluctuate for small $R$. The next lemma shows, however, that if we start out the Lorentz particle in a probability distribution $g(q,\Omega)\,dq\,d\Omega$ which is absolutely continuous with respect to the Lebesque measure, then the random variables $Q \mapsto \int_{\Lambda\times S^2} dq\,d\Omega\,g(q,\Omega)P_\alpha{}^R(q,\Omega)$ do not fluctuate any more as $R \to 0$.

**Lemma 2.** Let $g: \Lambda \times S^2 \to \mathbb{R}$ be integrable. Then the random variable $F_\alpha(Q) = \int_{\Lambda\times S^2} dq\,d\Omega\,g(q,\Omega)P_\alpha{}^Q(q,\Omega)$ on $\Gamma$ with measure $\mu^{(R)}$ converges in probability to $\int_{\Lambda\times S^2} dq\,d\Omega\,g(q,\Omega)P_\alpha(q,\Omega)$ as $R \to 0$, $\alpha = 1, 2$.

*Proof.* We note first that the average of the square of $F_2$ is

$$\int_{\Lambda\times S^2} dq\,d\Omega \int_{\Lambda\times S^2} d'q'\,d\Omega'\,g(q,\Omega)g(q',\Omega') \int_\Gamma d\mu^{(R)}(Q)\,P_2{}^Q(q,\Omega)P_2{}^Q(q',\Omega') \tag{35}$$

Consider now a Lorentz gas with two moving particles, one starting at $(q,\Omega)$, the other at $(q',\Omega')$. Then the third factor in (35) can be regarded as the probability of both particles being absorbed at the top wall $\{z = L\}$ before hitting the bottom wall $\{z = 0\}$. There are correlations between $P_2{}^Q(q,\Omega)$ and $P_2{}^Q(q',\Omega')$, since both particles may collide with the same scatterer. We now use the same techniques as in the proof of Lemma 1. If $(q, \Omega) \neq (q', \Omega')$, we consider only those paths for which both particles are absorbed at $\{z = L\}$ and for which there are no recollisions (one particle collides with the same scatterer more than once) and no double collisions (both particles collide with the same scatterer). Then, repeating the arguments in the proof of Lemma 1, this sum converges to $P_2(q, \Omega)P_2(q', \Omega')$. Considering also the combinations 11, 12, 21, the contribution of the remaining paths has by normalization to go to zero as $R \to 0$. Since $\{q = q'\} \times \{\Omega = \Omega'\}$ is a set of measure zero, we conclude that (35) converges to

$$\left[\int_{\Lambda \times S^2} dq\, d\Omega\, g(q, \Omega) P_2(q, \Omega)\right]^2$$

as $R \to 0$, i.e., $\langle F_2 \rangle - \langle F_2 \rangle^2 \to 0$ as $R \to 0$ and so the lemma is proved. ■

We combine Lemmas 1 and 2 to obtain the main result of our investigation.

**Theorem.** Let $f^{(R)}$ be the stationary state of the Lorentz gas [cf. (9)] and let $f$ be the stationary state of the linear Boltzmann equation [cf. (12)]. Then

$$\lim_{R \to 0} \int_{\Lambda \times \mathbb{R}^3} dq\, dp\, |f^{(R)}(q, p) - f(q, p)| = 0 \tag{36}$$

i.e., $f^{(R)}$ converges to $f$ in the $L^1$-norm. Furthermore, let $g : \Lambda \times \mathbb{R}^3 \to \mathbb{R}$ be bounded and measurable. Then the random variable

$$Q \mapsto \int_{\Lambda \times \mathbb{R}^3} dq\, dp\, g(q, p) f^Q(q, p)$$

on $\Gamma$ with measure $\mu^{(R)}$ [cf. (7)] converges in probability to

$$\int_{\Lambda \times \mathbb{R}^3} dq\, dp\, g(q, p) f(q, p)$$

*Proof.* By Lemma 2, $Q \to N(Q)$ converges in probability to $N$. Therefore $\mu^{(R)}(\Gamma_0) \to 1$ as $R \to 0$. Given $\epsilon \to 0$, we can find a small enough $R$ such that $\Gamma_0$ can be partitioned into $\Gamma_0' \cup \Gamma_0''$ in such a way that $\mu^{(R)}(\Gamma_0'') < \epsilon$, $\mu^{(R)}(\Gamma_0') > 1 - 2\epsilon$, and $|N(Q) - N| < \epsilon$ for all $Q \in \Gamma_0'$. Therefore

$$\begin{aligned}
\frac{1-\epsilon}{N+\epsilon} \int_{\Gamma_0'} d\mu^{(R)}(Q) \Big[\sum_{\alpha=1}^{2} \rho_\alpha(p) P_\alpha^Q(q, \Omega) &+ (1-\epsilon) \int_{\Gamma_0''} d\mu^{(R)}(Q) f^Q(q, p) \\
&\leqslant f^{(R)}(q, p) \\
&\leqslant \frac{1+\epsilon}{N-\epsilon} \int_{\Gamma_0'} d\mu^{(R)}(Q) \left[\sum_{\alpha=1}^{2} \rho_\alpha(p) P_\alpha^Q(q, \Omega)\right] \\
&\quad + (1+\epsilon) \int_{\Gamma_0''} d\mu^{(R)}(Q) f^Q(q, p)
\end{aligned} \tag{37}$$

Using the normalization of $f^{(R)}$ and $f$, we conclude that

$$\int_{\Lambda \times \mathbb{R}^3} dq\, dp \int_{\Gamma_0''} d\mu^{(R)}(Q) f^Q(q, p) < \epsilon c \tag{38}$$

with an appropriate constant $c$.

The condition (38) combined with Lemma 1 and (37) implies the $L^1$-convergence of $f^{(R)}$ as $R \to 0$. The second assertion of the theorem is an immediate consequence of Lemma 2. ∎

Let us work out what the theorem tells us about the heat flow in the Lorentz gas. We consider the steady-state heat flux $J^Q(q; L)$ at $q$ as a random variable on $\Gamma$ with measure $\mu^{(R)}$ [cf. (10)]. Although the second part of the theorem does not strictly apply, the argument used in the proof of Lemma 2 shows that $J^Q(q; L)$ does not fluctuate in the limit as $R \to 0$. Therefore, for a fixed $L$, given any $\epsilon > 0$, we can find an $R'$ sufficiently small such that for $R \leqslant R'$

$$|J^Q(q; L) - J(q; L)| < \epsilon/L$$

for all configurations $Q$ in a set $\Gamma^0$ of measure $\mu^{(R)}(\Gamma^0) > 1 - \epsilon$, i.e., up to a set of measure $\epsilon$, the difference in the heat conductivities $|\kappa^Q(q; L) - \kappa(q; L)|$ is bounded by $\epsilon$. Furthermore, in the case where $\rho_\alpha$ is a Maxwellian corresponding to temperature $T_\alpha$, $\alpha = 1, 2$, by Section 3, for $L \gg \rho^{-1}$, $\kappa(q; L)$ is independent of $L$ and $q$ and given by

$$\frac{8}{3}\left(\frac{2}{\pi}\right)^{1/2} \frac{(T_1 T_2)^{1/2}}{\sqrt{T_1} + \sqrt{T_2}} \rho^{-1}$$

## 5. COMMENTS

(i) More general stochastic boundary conditions: A real gas–surface interaction can be more complicated than assumed here.[4] Therefore, it is useful to notice that our results remain valid for a more general class of stochastic boundary conditions. If we denote by $K_q^\alpha(dp'|p)$, $\alpha = 1, 2$, the transition probability at the point $q$ of the $\alpha$th surface, then we assumed in this paper $K_q^\alpha(dp'|p) = (1/\pi)|e \cdot p'|\rho_\alpha(p')\, dp'$. Going back to the boundary condition (5), we observe that $f^Q$ is still stationary, if we assume that the kernel $K_q^\alpha(dp'|p)$ is given by the transition density

$$k_q^\alpha(v'|v)(v')^2\, dv'\, \bar{k}_q^\alpha(\Omega'|\Omega)\, d\Omega'$$

with the properties

$$\int_0^\infty dv\, k_q^\alpha(v'|v) v^3 \rho_\alpha(v) = v' \rho_\alpha(v'), \qquad \alpha, \beta = 1, 2$$

$$\int_{\{e \cdot \Omega \leqslant 0\}} d\Omega\, \bar{k}_q^\alpha(\Omega'|\Omega)|\cos\theta| = |\cos\theta'|, \qquad e \cdot \Omega' \geqslant 0 \tag{39}$$

(ii) Smooth potentials: The validity of Fourier's law should be independent of the details of the microscopic scattering. Therefore, we describe in some detail how to extend our analysis to the case of randomly distributed scatterers with a smooth potential. (The extension to a potential with hard core together with a smooth part is then obvious.)

First, we study the construction of a stationary measure for a fixed configuration $Q$ of scatterers. Let $V: \mathbb{R}^3 \to \mathbb{R}$ be a twice differentiable central potential of range 1 and let $V_R(q) = V(q/R)$. For a given configuration $Q$ of scatterers, $T_t^Q$ is now the flow generated by the Hamiltonian

$$H^Q = \frac{p^2}{2} + \sum_{i=1}^{j} V_R(q - Q_i), \qquad Q = (Q_1, ..., Q_j) \tag{40}$$

together with specularly reflecting boundary conditions. At the top and bottom wall we assume the same stochastic boundary conditions as in Section 2. To avoid notational complications the scatterers are not allowed to touch either the top or bottom wall. A stationary density $f^Q(q, p)$ still has to satisfy the conditions 1–3 of Section 2.

In contrast to the hard-sphere case, the absorption probabilities will now depend on $|p|$. Therefore we cannot find the solution to (4) by inspection. In fact, we cannot even guarantee the existence of a solution at all. (There are general theorems for Markov processes assuring the existence of a stationary probability measure absolutely continuous with respect to some given measure.[23,24] Unfortunately, the assumptions of those theorems are not so easily checked for the case at hand.) There is, however, a way out which, although mathematically not quite so appealing, is physically acceptable. The basic idea is to discretize the emission probabilities. For this purpose we choose a finite partition $\{\Delta_{1,m}\}_{m=1}^{M_1}$ of the bottom wall and a finite partition $\{\Delta_{2,m}\}_{m=1}^{M_2}$ of the top wall. We assume the following new stochastic boundary conditions: If the particle arrives at the $\alpha$th wall in $\Delta_{\alpha,m}$, then , independent of its incoming velocity and position of arrival in $\Delta_{\alpha,m}$, it is emitted uniformly spread out over $\Delta_{\alpha,m}$ with velocity distribution $\rho_\alpha(p) \max(0, e \cdot p)\, dp$.

The boundary values of the stationary density $f^Q$ have to be of the form

$$f^Q(x, y, (\alpha - 1)L, p) = g_{\alpha,m}(Q)\rho_\alpha(p), \qquad \alpha = 1, 2 \tag{41}$$

for $(x, y) \in \Delta_{\alpha,m}$, $e \cdot p \geqslant 0$, with nonnegative constants $g_{\alpha,m}(Q)$ to be determined. Let

$$K^Q(\alpha, m|\beta, n) = |\Delta_{\alpha,m}|^{-1} \int_{\Delta_{\alpha,m}} dx\, dy \int_0^\infty dv \int_{\{e\cdot\Omega\leqslant 0\}} d\Omega \times v^3 \cos\theta\, \rho_\beta(v) P_{\text{abs}}^Q(\Delta_{\beta,n}|x, y, (\alpha - 1)L, p) \tag{42}$$

Inserting (41) in (4), we obtain

$$g_{\alpha,m}(Q) = \sum_{\beta=1}^{2} \sum_{n=1}^{M_\beta} K^Q(\alpha, m|\beta, n) g_{\beta,n}(Q) \tag{43}$$

Since $K^Q(\alpha, m|\beta, n) \geqslant 0$ and $\sum_{\beta=1}^{2} \sum_{n=1}^{M_\beta} K^Q(\alpha, m|\beta, n) = 1$, $K^Q$ is a finite-dimensional stochastic matrix and (43) always has a solution, also denoted by $g_{\alpha,m}(Q)$. The simplicity of hard-sphere scatterers stems from the fact that in this case $K^Q$ is doubly stochastic, which implies that $g_{\alpha,m}(Q) = 1$ is always a solution. Let

$$P^Q_{\alpha,m}(q, p) = P^Q_{\text{abs}}(\Delta_{\alpha,m}|q, p) \tag{44}$$

Then, as in Section 2, the stationary solution $f^Q$ is given by

$$f^Q(q, p) = N(Q)^{-1} \sum_{\alpha=1}^{2} \sum_{m=1}^{M_\alpha} g_{\alpha,m}(Q) \rho_\alpha(p) P^Q_{\alpha,m}(q, p) \tag{45}$$

with suitable normalization constant $N(Q)$. Again, we define the stationary distribution $f^{(R)}(q, p)$ as the average of (45) over the Poisson distribution.

In the Boltzmann–Grad limit, $R \to 0$, the time evolution of the Lorentz gas is described by a linear Boltzmann equation, where the collision term is now

$$v\rho\left\{\int_{S^2} \sigma(d\Omega'|\Omega) f(q, \Omega', v, t) - f(q, \Omega, v, t)\right\}$$

$\sigma(d\Omega'|\Omega)$ is the differential cross section of the potential $V$, i.e., the probability of being scattered in direction $d\Omega'$ given a uniform incident beam in direction $\Omega$. One can show that there is a unique stationary solution $f(q, p)$ satisfying the stochastic boundary conditions. If $L \gg \rho^{-1} \times$ (degree of forward scattering), then Fourier's law is valid.

The convergence of $f^{(R)}$ as $R \to 0$ is now more difficult to handle. The crucial fact is: The absorption probabilities $\int d\mu^{(R)}(Q)\, P^Q_{\alpha,m}(q, p) = P^{(R)}_{\alpha,m}(q, p)$ converge pointwise to the corresponding absorption probabilities $P_{\alpha,m}(q, p)$ of the linear Boltzmann equation and the "smeared out" absorption probabilities $\int dq\, dp\, P^Q_{\alpha,m}(q,p)\psi(q,p)$ converge in probability to $\int dq\, dp P_{\alpha,m}(q,p)\psi(q,p)$. (The proof is analogous to those of Lemmas 1 and 2.)

We note that the matrix elements of $K^Q$ are of the form

$$\int dq\, dp\, P^Q_{\alpha,m}(q, p)\psi(q, p)$$

for some $\psi$. Therefore $K^Q$ converges in probability to $K$ and

$$\lim_{R\to 0} \int d\mu^{(R)}(Q)\, g_{\alpha,m}(Q) = \sum_{\beta=1}^{2} \sum_{n=1}^{M_\beta} K(\alpha, m|\beta, n) \lim_{R\to 0} \int d\mu^{(R)}(Q)\, g_{\beta,n}(Q) \tag{46}$$

Let $g_{\alpha,m}$ be the solution of (46). One checks that $g_{\alpha,m}(Q)$ converges in probability to $g_{\alpha,m}$ as $R \to 0$. As before, $N(Q)$ converges to $N$ in probability as $R \to 0$. Now, we have the same situation as in the proof of the theorem. By the same argument we conclude then that $f^{(R)}$ converges to $f$ in the $L^1$-norm as $R \to 0$. Expectations in the stationary state converge in probability.

We summarize: The theorem is valid for scatterers with a twice differentiable central potential $V_R(q) = V(q/R)$ with $V$ of range 1.

(iii) Diffusion. In this paper we concentrated on the heat flow. But our method is also applicable to diffusion—in fact, diffusion is considerably easier to handle, in particular for scatterers with a smooth potential.

We consider a slab of thickness $L$ of random scatterers parallel to the $x$–$y$ plane. ($B$ is now the entire $x$–$y$ plane!) From the bottom there is an incident beam with speed $v$ and uniform angular distribution. We assume complete absorption for a particle leaving the slab. (We can easily build a strictly mechanical model corresponding to these boundary conditions: We fill the half-space $\{z < 0\}$ with an infinitely extended ideal gas with a constant density and velocity distribution corresponding to the incident beam. Whenever a particle leaves the strip $\{0 \leqslant z \leqslant L\}$ it moves freely.) Then the stationary distribution in the slab is simply $cP_1^{(R)}(q, \Omega; L)\, dq\, d\Omega$, where $c$ is a constant depending on the density of the incident beam. Therefore the stationary density is given by

$$n^{(R)}(q; L) = c \int_{S^2} d\Omega\, P_1^{(R)}(q, \Omega; L) \tag{47}$$

and the steady current at the point $q$ through a cross-sectional area parallel to the $x$–$y$ plane is given by

$$j^{(R)}(q; L) = cv \int_{S^2} d\Omega \cos\theta\, P^{(R)}(q, \Omega; L) \tag{48}$$

We expect for large $L$

$$j^{(R)}(q; L) = bD^{(R)}(1/L) \tag{49}$$

with $b$ some constant independent of $R$ and $L$.

By Lemma 1, in the Boltzmann–Grad limit, $R \to 0$, $n^{(R)}(q; L)$ converges to $n(q; L)$, and $j^{(R)}(q; L)$ converges to $j(q; L)$, where $n(q; L)$ and $j(q; L)$ are given by the stationary solution of the linear Boltzmann equation with the boundary conditions specified above. By (13) and (14), for $L \gg \rho^{-1}$, we obtain

$$j(q; L) = \frac{4\pi}{3} \frac{v}{\rho L}, \qquad n(q; L) = c4\pi \frac{L - z}{L} \tag{50}$$

According to Fick's law, $j(q) = -D\,\nabla n(q)$, which yields the diffusion constant $D = \frac{1}{3}v\rho^{-1}$. Therefore for finite $R$ we are led by (49) to *define* the diffusion constant as

$$D^{(R)} = \lim_{L\to\infty} \frac{1}{4\pi c} L_j^{(R)}(q; L)$$

$$= \lim_{L\to\infty} \frac{vL}{4\pi} \int_{S^2} d\Omega \cos\theta\, P_1^{(R)}(q, \Omega; L) \qquad (51)$$

This limit should exist and be independent of $q$.

On the other hand, as is well known,[25] the diffusion constant should be related to the time integral over the velocity autocorrelation function. One considers an infinitely extended Lorentz gas, i.e., a uniform distribution of scatters over the whole space, and argues that, if the Lorentz particle starts with a uniform velocity distribution and a fixed speed $v$, then the mean square displacement $\langle [q(t) - q]^2 \rangle_{(R)}$ should behave as $6D^{(R)}t$ for large $t$ as expected from the diffusion equation. Here, $\langle \cdot \rangle_{(R)}$ denotes the average over the Poisson distribution of scatterers of radius $R$ and over the initial velocity distribution $(1/4\pi)\, d\Omega$. This leads then immediately to

$$D^{(R)} = \lim_{T\to\infty} \tfrac{1}{3} \int_0^T dt\, \langle p(t)\cdot p \rangle_{(R)}$$

$$= \lim_{T\to\infty} \int_0^T dt\, \langle (\cos\theta(t) \cos\theta \rangle_{(R)} v^2 \qquad (52)$$

For the linear Boltzmann equation, (51) and (52) give the same answer. We expect this to be true also for finite $R$. However, even by formal manipulations we were unable to check the conjectured identity.

In most numerical experiments,[26–28] trying to obtain $D^{(R)}$ by computer simulations, and in theoretical studies,[18,28,30] trying to obtain series expansions for $D^{(R)}$, the starting point is (52). However, (51) seems to be closer to how one actually measures a diffusion constant and appears to be as accessible to numerical studies as (52). Indeed one investigation of this type was done by Visscher.[31] More investigations in this direction would be of great interest.

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