The existence of Burnett coefficients in the periodic Lorentz gas

N. I. Chernov* and C. P. Dettmann†

October 6, 1999

Abstract

The linear super-Burnett coefficient gives corrections to the diffusion equation in the form of higher derivatives of the density. Like the diffusion coefficient, it can be expressed in terms of integrals of correlation functions, but involving four different times. The power law decay of correlations in real gases (with many moving particles) and the random Lorentz gas (with one moving particle and fixed scatterers) are expected to cause the super-Burnett coefficient to diverge in most cases. Here we show that the expression for the super-Burnett coefficient of the periodic Lorentz gas converges as a result of exponential decay of correlations and a nontrivial cancellation of divergent contributions.

1 Introduction

To leading order, the equations of hydrodynamics describe the transport of microscopically conserved quantities supplemented by linear constitutive relations between the relevant thermodynamic forces and fluxes. For example, the conservation of the number of particles of a light species moving in an arrangement of fixed scatterers is described macroscopically using the continuity equation

$$\frac{\partial n}{\partial t} = -\nabla \cdot \mathbf{J} \tag{1}$$

relating the number density n to the current $\mathbf{J}$. Under a hydrodynamic approximation where n is "smooth", hence all of its derivatives are small, the flux $\mathbf{J}$ is given as a linear function of the force ∇n, that is, in an isotropic homogeneous medium,

$$\mathbf{J} = -D\nabla n \tag{2}$$

*Department of Mathematics, University of Alabama at Birmingham, Birmingham, AL 35294.
†Center for Studies in Physics and Biology, Rockefeller University, New York, NY 10021.

leading to the diffusion equation

$$\frac{\partial n}{\partial t} = D\nabla^2 n \tag{3}$$

where D is the diffusion coefficient. Similar considerations involving energy and momentum conservation lead to the Navier-Stokes equations for a fluid.

There have been many attempts to go beyond this leading hydrodynamic approximation. The constitutive relation can contain an expansion in terms of higher derivatives of the forces and/or higher powers of the forces. In the former case one talks of linear Burnett [3] coefficients, and in the latter, of nonlinear Burnett coefficients. The first correction in either case (coefficient of $\nabla^2 n$ or $(\nabla n)^2$) is often called a Burnett coefficient and the second correction (coefficient of $\nabla^3 n$ or $(\nabla n)^3$) a super-Burnett coefficient, and so on. We consider the Lorentz gas, in which the light particles do not mutually interact, so only linear relations are possible. In addition, it is equally likely for a particle to move in one direction or the opposite direction, so the $\nabla^2 n$ term cancels and we are left with the linear super-Burnett coefficient. We will dispense with this cumbersome terminology and call it simply the Burnett coefficient.

Using the Boltzmann equation, hence a limit in which all collisions are uncorrelated, the Chapman-Enskog method allows the computation of D as well as other and higher order transport coefficients of a low density gas. One of the greatest surprises of nonequilibrium kinetic theory was the discovery [7] that density corrections due to recollisions of several particles diverge. This leads to a nonanalytic dependence of transport coefficients on density in the case of the random Lorentz gas [11], where noninteracting point particles collide with a random arrangement of non-overlapping hard spheres in two or three dimensions, but not in an exactly solvable one dimensional model [10].

Subsequently the divergences were related to a power law decay of correlations (see [8] and references therein), the "long time tails", which are due to density fluctuations in infinite random systems. Since transport coefficients can be computed using integrals of correlation functions (see below), a slow decay of correlations can lead to divergences. As discussed in a review of random Lorentz models [1], the diffusion coefficient is typically defined, but Burnett coefficients may not be since the latter have more divergent expressions in general. The degree of divergence is greater for real gases than for Lorentz gases, and decreases with the dimension of the system. Here we show that, as a result of the exponential decay of correlations in the periodic Lorentz model, the combination of four-time correlation functions used to compute the Burnett coefficient decays sufficiently rapidly to ensure convergence. Thus a Burnett coefficient is defined for a random Lorentz gas in a dilute approximation and for a periodic Lorentz gas under general conditions.

2 The Burnett coefficient

Our notation follows that of Gaspard [9] who gives an account of deterministic diffusion including expressions for the Burnett coefficients. He suggests stretched exponential bounds on the four time correlations which we find, but does not give the precise form or rigorous proof.

We consider a periodic Lorentz gas in which a point particle moving with unit velocity undergoes specular reflections with a periodic array of scatterers. We consider only the case of finite horizon, so that time between collisions is bounded. The most usual case is that of circular scatterers in a hexagonal lattice, but we demand only that the scatterers be convex and sufficiently smooth, specifically C^3. We allow for any dimension $d \geq 2$, but note that a single spherical scatterer per unit cell cannot satisfy the finite horizon condition for $d > 2$. Thus we need either nonspherical scatterers or more than one per unit cell when $d > 2$.

Because the scatterers lie on a periodic lattice, it is possible to represent the dynamics in terms of a map $\boldsymbol{\phi}$ acting at the surface of the scatterers. We denote the position and velocity direction at the surface of a scatterer in the elementary cell by $\mathbf{x}$. Then the lattice translation vector $\mathbf{a}(\mathbf{x})$ gives the lattice displacement associated with the free flight following a collision at $\mathbf{x}$; this is a linear combination of the lattice basis vectors $\mathbf{e}^{(\alpha)}$ ($\alpha = 1 \ldots d$) with integer coefficients and is a piecewise constant function of $\mathbf{x}$. $T(\mathbf{x})$ is the time for this free flight. We can compute time averages, which for almost all initial conditions are equivalent to the natural measure on the surface of the scatterers $\langle\rangle$ due to ergodicity. We define $\Delta T(\mathbf{x}) = T(\mathbf{x}) - \langle T \rangle$ so that $\langle \Delta T \rangle = 0$. We use Greek indices to refer to spatial components such as a_α, and Latin indices to refer to collisions, with the shorthand notation $a_\alpha^i = a_\alpha(\boldsymbol{\phi}^i \mathbf{x})$ and $\Delta T^i = \Delta T(\boldsymbol{\phi}^i \mathbf{x})$. We have $\langle a_\alpha^i \rangle = 0$ and also odd combinations such as $\sum_{ij=-\infty}^{\infty} \langle a_\alpha^0 a_\beta^i a_\gamma^j \rangle = 0$ since time reversibility and phase space volume conservation imply that there are equal and opposite contributions from time reversed trajectory segments.

The general periodic Lorentz gas is homogeneous but not isotropic at large scales, so the hydrodynamic equation contains transport coefficients that are fully symmetric tensors, but do not depend on position:

$$\frac{\partial n}{\partial t} = D_{\alpha\beta} \nabla_\alpha \nabla_\beta n + B_{\alpha\beta\gamma\delta} \nabla_\alpha \nabla_\beta \nabla_\gamma \nabla_\delta n + \ldots \quad . \tag{4}$$

where $B_{\alpha\beta\gamma\delta}$ are the Burnett coefficients and repeated Greek indices are summed. A general solution can be obtained with a Fourier-Laplace transform of the form $n \sim \exp(st + i\mathbf{k} \cdot \mathbf{r})$ leading to a dispersion relation

$$s(\mathbf{k}) = -D_{\alpha\beta} k_\alpha k_\beta + B_{\alpha\beta\gamma\delta} k_\alpha k_\beta k_\gamma k_\delta + \ldots \tag{5}$$

The Green-Kubo relations for the transport coefficients in terms of integrals (sums) of correlation functions are given in continuous time in, for example, Ref. [1], and in discrete time [9] they are

$$D_{\alpha\beta} = \frac{1}{2\langle T \rangle} \sum_{i=-\infty}^{\infty} \langle a_\alpha^0 a_\beta^i \rangle \tag{6}$$

and

$$B_{\alpha\beta\gamma\delta} \;=\; \frac{1}{24} [F_{\alpha\beta\gamma\delta} + 4C(D_{\alpha\beta} D_{\gamma\delta} + D_{\alpha\gamma} D_{\beta\delta} + D_{\alpha\delta} D_{\beta\gamma}) \tag{7}$$

$$-2(D_{\alpha\beta}E_{\gamma\delta}+D_{\alpha\gamma}E_{\beta\delta}+D_{\alpha\delta}E_{\beta\gamma}+D_{\beta\gamma}E_{\alpha\delta}+D_{\beta\delta}E_{\alpha\gamma}+D_{\gamma\delta}E_{\alpha\beta})]$$

with

$$C = \frac{1}{\langle T\rangle}\sum_{i=-\infty}^{\infty}\langle \Delta T^0 \Delta T^i\rangle \tag{8}$$

$$E_{\alpha\beta} = \frac{1}{\langle T\rangle}\sum_{i,j=-\infty}^{\infty}\langle \Delta T^0 a_\alpha^i a_\beta^j\rangle \tag{9}$$

$$\begin{aligned} F_{\alpha\beta\gamma\delta} &= \frac{1}{\langle T\rangle}\sum_{i,j,k=-\infty}^{\infty}\Big[\langle a_\alpha^0 a_\beta^i a_\gamma^j a_\delta^k\rangle - \langle a_\alpha^0 a_\beta^i\rangle\langle a_\gamma^j a_\delta^k\rangle \\ &\quad -\langle a_\alpha^0 a_\gamma^j\rangle\langle a_\beta^i a_\delta^k\rangle - \langle a_\alpha^0 a_\delta^k\rangle\langle a_\beta^i a_\gamma^j\rangle\Big] \end{aligned} \tag{10}$$

It is possible to make the lower limits of the sums all zero with some extra symmetrization and special treatment of the zero terms. The convergence of the sum for C follows in a straightforward manner from the known exponential decay of correlations in this system [6]. The convergence of the sum for $E_{\alpha\beta}$ follows from Theorem 3 in the following section. The sum for $F_{\alpha\beta\gamma\delta}$ is still less clear since each term diverges; however Theorem 1 in the following section show that the combination converges, leading to finite Burnett coefficients.

In the case of the hexagonal Lorentz gas, the six-fold rotational symmetry is sufficient to restrict the coefficients to their isotropic forms $D_{\alpha\beta}=D\delta_{\alpha\beta}$ and $B_{\alpha\beta\gamma\delta}=B(\delta_{\alpha\beta}\delta_{\gamma\delta}+\delta_{\alpha\gamma}\delta_{\beta\delta}+\delta_{\alpha\delta}\delta_{\beta\gamma})/3$. It seems likely that a straightforward application of our results could also show the existence of the higher order Burnett coefficients, for which there exist long expressions similar to those given here. In this case it would be interesting to consider the radius of convergence of Eq. (5).

3 Proofs

The billiard map $\boldsymbol{\phi}$ is defined on the collision space M of the periodic Lorentz gas. In the case of finite horizon, the map $\boldsymbol{\phi}$ and the above functions a_α and ΔT are piecewise Hölder continuous [2, 4]. This means that M can be partitioned into finitely many domains with piecewise smooth boundaries on each of which the function is Hölder continuous.

We always denote by $\langle\cdot\rangle$ the integration over M with respect to the invariant equilibrium measure. In all theorems below, $f_0, f_1, \ldots$ denote piecewise Hölder continuous functions on M such that $\langle f_k\rangle = 0$ for all k. For $i\geq 0$ we put $f_k^i = f_k\circ\boldsymbol{\phi}^i$.

Theorem 1 *The following series*

$$\sum_{i_1,i_2,i_3=0}^{\infty}\langle f_0^0 f_1^{i_1} f_2^{i_2} f_3^{i_3}\rangle - \langle f_0^0 f_1^{i_1}\rangle\langle f_2^{i_2} f_3^{i_3}\rangle - \langle f_0^0 f_2^{i_2}\rangle\langle f_1^{i_1} f_3^{i_3}\rangle - \langle f_0^0 f_3^{i_3}\rangle\langle f_1^{i_1} f_2^{i_2}\rangle \tag{11}$$

always converges absolutely.

We prove general estimates on multiple correlation functions, from which the above theorem will follow.

Theorem 2 *Let $i_1 \le \cdots \le i_k$ and $1 \le t \le k-1$. Then*

$$|\langle f_1^{i_1} \cdots f_k^{i_k} \rangle - \langle f_1^{i_1} \cdots f_t^{i_t} \rangle \langle f_{t+1}^{i_{t+1}} \cdots f_k^{i_k} \rangle| \le C_k \cdot |i_k - i_1|^2 \, \lambda^{|i_{t+1}-i_t|^{1/2}} \tag{12}$$

where $C_k > 0$ depends on the functions $f_1, \ldots, f_k$, and $\lambda < 1$ is independent of k and $f_1, \ldots, f_k$.

This allows us to "decouple" multiple correlations provided the gap between the time moments i_t and i_{t+1} is long enough.

Remark. In view of recent advances in the study of correlations for billiard dynamics [12, 6] it is very likely that the above estimate can be upgraded to $C_k \lambda^{|i_{t+1}-i_t|}$ for some $\lambda < 1$, which would be an exponential decay of (multiple) correlations. However, the estimate (12) is easier to prove, and for our purposes it is good enough.

We postpone the proof of the Theorem 2 and first obtain Theorem 1 and other interesting implications.

Theorem 3 *Let $i_1 \le \cdots \le i_k$. Consider the $k-1$ differences $m_t = i_{t+1} - i_t$ for $1 \le t \le k-1$. Let $m_{(1)} \le m_{(2)} \le \cdots \le m_{(k-1)}$ be the ordered differences $m_1, \ldots, m_{k-1}$. Let $m = m_{(r)}$ where $r = [(k+1)/2]$. Then*

$$|\langle f_1^{i_1} \cdots f_k^{i_k} \rangle| \le C_k \cdot |i_k - i_1|^2 \, \lambda^{m^{1/2}}$$

where $C_k > 0$ and $\lambda < 1$ (here λ is the same as in the previous theorem).

To prove this theorem, we use a simple lemma:

Lemma 4 *Let $k \ge 2$ and $r = [(k+1)/2]$. If we partition k objects into $k-r+1$ nonempty groups, then at least one group contains exactly one object.*

Now, Theorem 3 is proved by applying Theorem 2 to the $k-r$ largest gaps $m_{(k-1)}, \ldots, m_{(r)}$ and recalling that $\langle f_j \rangle = 0$ for every j.

Note that there is no similar bound on multiple correlations in terms of the next difference, $m_{(r+1)}$. Indeed, no matter how large $m_{(r+1)}$ is, we can always arrange the time moments $i_1, \ldots, i_k$ so that $i_1 = i_2$, $i_3 = i_4$, …, $i_{k-1} = i_k$, and then the correlation $\langle f_1^{i_1} \cdots f_k^{i_k} \rangle$ need not be even small, in general it will stay bounded away from zero.

Corollary 5 *For $k = 2$, we obtain the known [2] bound on the 2-correlation function:*

$$|\langle f_1^{i_1} f_2^{i_2} \rangle| \le C(f_1, f_2) \cdot \lambda_0^{|i_2-i_1|^{1/2}}$$

for some $C(f_1, f_2) > 0$ and $\lambda_0 < 1$.

We now prove Theorem 1. We can assume that $i_1 \le i_2 \le i_3$ in (11) and put $\bar{m} = \max\{i_1, i_2 - i_1, i_3 - i_2\}$. Then it easily follows from Theorem 2 and the above corollary that

$$|\langle f_0^0 f_1^{i_1} f_2^{i_2} f_3^{i_3}\rangle - \langle f_0^0 f_1^{i_1}\rangle\langle f_2^{i_2} f_3^{i_3}\rangle - \langle f_0^0 f_2^{i_2}\rangle\langle f_1^{i_1} f_3^{i_3}\rangle - \langle f_0^0 f_3^{i_3}\rangle\langle f_1^{i_1} f_2^{i_2}\rangle| \le C\,\bar{m}^2\lambda^{\bar{m}^{1/2}}$$

This easily implies the absolute convergence of the series (11). Theorem 1 is proved.

Theorem 6 *Let $S_n = f_0^0 + f_0^1 + \cdots + f_0^{n-1}$. Then the k-th moment of S_n can be bounded by*

$$|\langle S_n^k\rangle| \le C(f_0, k)\cdot n^{[k/2]}$$

where $C(f_0, k) > 0$.

This theorem follows from Theorem 3. In the case $k = 4$ see the proof in [2]. The argument generalizes to any $k \ge 3$ rather directly. In view of the remark made after Lemma 4, the above estimate cannot be improved, in general.

Proof of Theorem 2. We use the partition method developed in [2] and further enhanced in [5]. Note that [2, 5] discuss two-dimensional periodic Lorentz gases, but all the results hold in any dimensions as well [4]. We recall the essentials of the partition method in a more general setting than our Lorentz gas model.

Let $\boldsymbol{\phi} : M \to M$ be a measurable transformation of a metric space M preserving a nonatomic Borel probability measure μ. Let $\mathcal{A} = \{A_1, A_2, \ldots\}$ be a finite or countable measurable partition of M, we denote $\operatorname{diam}\mathcal{A} = \sup_i\{\operatorname{diam} A_i\}$. We put $\mathcal{A}_n = \boldsymbol{\phi}^{-n}\mathcal{A} = \{\boldsymbol{\phi}^{-n}A_i\}$ for $n \ge 0$ and $\mathcal{A}_{n,k} = \mathcal{A}_n \vee \cdots \vee \mathcal{A}_k$ for $k \ge n \ge 0$. A measure of dependence between two partitions $\mathcal{A} = \{A_i\}$ and $\mathcal{B} = \{B_j\}$ of the space M is defined to be

$$\beta(\mathcal{A}, \mathcal{B}) = \sum_{i,j} |\mu(A_i \cap B_j) - \mu(A_i)\mu(B_j)|$$

Based on this measure, we put

$$\beta_N(n) = \max_{0 \le k \le N-n-1} \beta(\mathcal{A}_{0,k}, \mathcal{A}_{k+n,N-1}), \tag{13}$$

for any $N \ge n \ge 0$. Note that $\beta_N(n)$ is called the mixing coefficients of the partition $\mathcal{A}$, cf. [5].

For any measurable bounded function f on M and a partition $\mathcal{A}$ of M we denote $\bar{f}_{\mathcal{A}} = \langle f|\mathcal{A}\rangle$ the conditional expectation of f with respect to the σ-algebra generated by $\mathcal{A}$, and $\Delta_{\mathcal{A}} f = f - \bar{f}_{\mathcal{A}}$. We put

$$\mathcal{H}_f(d) = \sup_{\operatorname{diam}\mathcal{A} \le d} ||\Delta_{\mathcal{A}} f||_2$$

Clearly, $\mathcal{H}_f(d)$ monotonically decreases to zero as $d \to 0$, and the speed of decrease characterizes the "smoothness" of f, see [5] and below.

Lemma 7 *For any functions $f_1, \ldots, f_k$ on M and any partition $\mathcal{A}$ with $d = \operatorname{diam} \mathcal{A}$ we have*

$$|\langle f_1^{i_1} \cdots f_k^{i_k} \rangle - \langle f_1^{i_1} \cdots f_t^{i_t} \rangle \langle f_{t+1}^{i_{t+1}} \cdots f_k^{i_k} \rangle| \le C_k \left[\sum_{t=1}^{k} \mathcal{H}_{f_t}(d) + \beta_{i_k - i_1}(i_{t+1} - i_t) \right] \qquad (14)$$

Proof. First, we replace f_t by $\bar{f}_t = \bar{f}_{t,\mathcal{A}}$. The error can be estimated by

$$|\langle f_1^{i_1} \cdots f_k^{i_k} \rangle - \langle \bar{f}_1^{i_1} \cdots \bar{f}_k^{i_k} \rangle| \le C_k \sum_t ||\Delta_{\mathcal{A}} f_t||_2 \le C_k \sum_t \mathcal{H}_{f_t}(d)$$

which is a simple calculation using Schwarz' inequality, cf. [5]. Two other correlations in (14) can be handled similarly.

Next, it is rather straightforward that

$$|\langle \bar{f}_1^{i_1} \cdots \bar{f}_k^{i_k} \rangle - \langle \bar{f}_1^{i_1} \cdots \bar{f}_t^{i_t} \rangle \langle \bar{f}_{t+1}^{i_{t+1}} \cdots \bar{f}_k^{i_k} \rangle| \le \prod_t ||f_t||_\infty \times \beta_{i_k - i_1}(i_{t+1} - i_t)$$

(for $k = 2$, this was done in [5], the general case is similar). Lemma is proved. $\square$

We now need a good partition $\mathcal{A}$ for our Lorentz gas map $\boldsymbol{\phi} : M \to M$. Such a partition was constructed in [2, 4] and further refined in [5]. Here we state the result:

Theorem 8 (see [5]) *Let $\boldsymbol{\phi} : M \to M$ be the billiard map for a periodic Lorentz gas with finite horizon. Then for any $N \ge m \ge 1$ there is a partition $\mathcal{A} = \mathcal{A}_{N,m}$ such that*
(i) $\operatorname{diam} \mathcal{A} \le c_1 \lambda_1^{m^{1/2}}$,
(ii) $\beta_N(m) \le c_2 N^2 \lambda_2^{m^{1/2}}$
for some constants $c_1, c_2 > 0$ and $\lambda_1, \lambda_2 < 1$.

It remains to estimate the term $\mathcal{H}_{f_t}(d)$ in (14). Let f be a piecewise Hölder continuous function on M. Then one can easily obtain [5] that $\mathcal{H}_f(d) \le C(f) \cdot d^\alpha$ for some $\alpha > 0$. Now Theorem 2 follows from Lemma 7 and Theorem 8.

Acknowledgements. CD is grateful for discussions with E. G. D. Cohen and J. R. Dorfman, and for the support of the Engineering Research Program of the Office of Basic Energy Sciences at the US Department of Energy, contract #DE-FG02-88-ER13847. NC is partially supported by NSF grant DMS-9732728.

References

[1] H. van Beijeren, *Transport properties of stochastic Lorentz models*, Rev. Mod. Phys. **54** (1982), 195–234.

[2] L.A. Bunimovich, Ya. G. Sinai, and N. I. Chernov, *Statistical properties of two-dimensional hyperbolic billiards*, Russ. Math. Surv. **46** (1991), 47–106.

[3] D. Burnett, *The distribution of molecular velocities and the mean motion in a non-uniform gas*, Proc. London Math. Soc. **40** (1935), 382–435.

[4] N. I. Chernov, *Statistical properties of the periodic Lorentz gas. Multidimensional case*, J. Stat. Phys. **74** (1994), 11–53.

[5] N. I. Chernov, *Limit theorems and Markov approximations for chaotic dynamical systems*, Prob. Th. Relat. Fields **101** (1995), 321–362.

[6] N. I. Chernov, *Decay of correlations and dispersing billiards*, J. Stat. Phys. **94** (1999), 513–556.

[7] J. R. Dorfman and E. G. D. Cohen, *On the density expansion of the pair distribution function for a dense gas not in equilibrium*, Phys. Lett. **16** (1965), 124–125.

[8] M. H. Ernst and A. Weyland, *Long time behaviour of the velocity autocorrelation function in a Lorentz gas*, Phys. Lett. A **34** (1971), 39–40.

[9] P. Gaspard, "Chaos, scattering and statistical mechanics", chapter 7 (Cambridge University Press, Cambridge UK, 1998).

[10] J. L. Lebowitz and J. Percus, *Kinetic equations and density expansions: Exactly solvable one-dimensional system*, Phys. Rev. **155** (1967), 122–138.

[11] J. M. J. van Leeuwen and A. Weijland, *Non-analytic density behaviour of the diffusion coefficient of a Lorentz gas*, Physica **36** (1967), 457–490.

[12] L.-S. Young, *Statistical properties of dynamical systems with some hyperbolicity*, Annals of Math. **147** (1998), 585–650.