The Burnett expansion of the periodic Lorentz gas

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Abstract

The macroscopic limit of some deterministic scattering processes can be described by the diffusion equation $\partial_t \rho = D\nabla^2\rho$, where the diffusion coefficient D is given by a sum over two-time correlation functions, the discrete time version of the Green-Kubo integral over the velocity autocorrelation function. The approximation can be improved by allowing higher spatial derivatives; in this case the coefficients are called Burnett coefficients, and are given by sums over multiple time correlation functions. The periodic Lorentz gas has exponential decay of two-time correlation functions, implying the existence of the diffusion coefficient. Recent work has established a stretched exponential decay of multiple correlation functions and the existence of the fourth order Burnett coefficient for the periodic Lorentz gas. Here we give expressions for the higher coefficients, show that these expressions converge, and give a plausible argument based on similar models that the expansion composed of the Burnett coefficients has a finite radius of convergence.

1 Introduction

The *Lorentz gas* is a model used in statistical mechanics, consisting of a point particle moving at constant velocity except for specular collisions with smooth (specifically C^3) convex fixed scatterers in $d \geq 2$ dimensions. The original model has randomly placed scatterers in infinite space, and is known to have power law decay of correlations, so that the Burnett coefficients (defined below as sums of such correlations) are not generally expected to exist [10]. Here we consider a periodic arrangement of scatterers which is equivalent to a dispersing billiard on a torus, so that two-time correlations (in discrete time) decay exponentially [11, 4]. This, together with the *finite horizon* condition, that is, that the time between collisions is bounded, implies the existence of the diffusion coefficient ($D^{(2)}$ below). A recent paper [5] gives a stretched exponential decay of multiple correlations [5], and uses this to show (again with finite horizon) that the fourth order Burnett coefficient ($D^{(4)}$ below) exists. Here we extend this result to all the Burnett

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coefficients. A common example for $d = 2$ with a finite horizon is given by circular scatterers on a hexagonal lattice; for $d > 2$ the finite horizon condition requires either nonspherical scatterers, or more than one scatterer per unit cell. The Lorentz gas and its various extensions are discussed extensively in Ref. [9].

From the point of view of statistical mechanics, the microscopic (Liouville or Frobenius-Perron) evolution of the probability density ρ of the particle in phase space $(\mathbf{r}, \mathbf{v})$ can be described using macroscopic or "hydrodynamic" equations in real space $\mathbf{r}$ at distance and time scales large with respect to the size of the scatterers, the periodic cell, and the time between collisions. The diffusion equation in a homogeneous but anisotropic medium corresponding to the periodic Lorentz gas is

$$\partial_t \rho = D^{(2)}_{\alpha\beta} \partial_\alpha \partial_\beta \rho \tag{1}$$

where the Greek indices indicate spatial dimensions, and repeated Greek indices are summed. One systematic improvement of the hydrodynamic approximation, suggested by Burnett [2], is the addition of higher spatial derivatives corresponding to smaller distance scales,

$$\partial_t \rho = D^{(2)}_{\alpha\beta} \partial_\alpha \partial_\beta \rho + D^{(4)}_{\alpha\beta\gamma\delta} \partial_\alpha \partial_\beta \partial_\gamma \partial_\delta \rho + \ldots \tag{2}$$

and the higher coefficients are called (linear) Burnett coefficients. Nonlinear terms such as powers of $\partial_\alpha \rho$ are excluded here because ρ is a projection onto real space of a phase space density satisfying a linear evolution equation. The presence of only even terms here and in Eq. (4) below is expected by symmetry arguments; we do not assume this until it is justified at the end of Sec. 2.

The solutions of the generalized diffusion equation are of the form

$$\rho(\mathbf{r}, t) = \exp(s(\mathbf{k})t + \mathrm{i}\mathbf{k} \cdot \mathbf{r}) \tag{3}$$

with a dispersion relation

$$s(\mathbf{k}) = -D^{(2)}_{\alpha\beta} k_\alpha k_\beta + D^{(4)}_{\alpha\beta\gamma\delta} k_\alpha k_\beta k_\gamma k_\delta + \ldots \tag{4}$$

describing the rate of exponential decay of the hydrodynamic mode corresponding to wave number $\mathbf{k}$. Note that the dispersion relation (4) may be a more convenient description than the generalized diffusion equation (2) when the Burnett coefficients do not exist, as $s(\mathbf{k})$ may still exist, but be nonanalytic.

The dispersion relation is obtained from the microscopic dynamics as discussed in chapter 7 of Ref. [7], from which we need only Eq. (7.91):

$$1 = \lim_{n \to \infty} \langle \prod_{i=-n}^{n-1} \exp\left[-s(\mathbf{k}) T(\boldsymbol{\phi}^i x) - \mathrm{i}\mathbf{k} \cdot \mathbf{a}(\boldsymbol{\phi}^i x) \right] \rangle \tag{5}$$

from which $s(\mathbf{k})$ can be obtained by an expansion in powers of $\mathbf{k}$. Here the billiard map $\boldsymbol{\phi}$ is defined on the collision space M, that is, $x = (\mathbf{r}, \mathbf{v}) \in M$ when $\mathbf{r}$ is on the boundary of one of the scatterers and $\mathbf{v}$ is in an outward direction from the scatterer. $T(x)$ is the time between the collision at x and the next; it is a piecewise Hölder continuous function [1, 3] (the finite horizon condition ensures that both T and $\mathbf{a}$ are bounded). $\mathbf{a}(x)$ is the lattice translation vector associated with this free flight; it is a linear combination of the lattice basis vectors $\mathbf{e}^{(\alpha)}$ with integer coefficients, and is a piecewise constant function. The average $\langle\cdot\rangle$ denotes integration over M with respect to the invariant equilibrium measure.

We are now in a position to state the main result of this paper:

Theorem 1 *The coefficients $D^{(m)}$ defined by a formal expansion of Eqs. (4,5) in powers of $\mathbf{k}$ are given by absolutely convergent series.*

The proof is in two parts. Sec. 2 shows how to expand the above expression to obtain the Burnett coefficients in terms of sums of correlation functions; we need only time reversibility and phase space volume conservation, so these expressions apply to more general periodic systems than the Lorentz gas. Sec. 3 uses the results of Ref. [5] together with some combinatorics to show that these series converge absolutely for the periodic Lorentz gas. The final section, Sec. 4 contains arguments in support of the following conjecture:

Conjecture 2 *The series defined by Eq.(4) has a finite radius of convergence.*

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2 Expressions for the Burnett coefficients

The coefficient $D^{(4)}$ is obtained in Ref. [7] by differentiating Eq. (5) with respect to $\mathbf{k}$ four times; the calculation is described as "long but straightforward". Here we are not interested in the explicit expressions obtained but rather their structure. We remark however, that the equations given here contain enough details to obtain the full expression for $D^{(6)}$ etc. efficiently if required.

We begin by noting that Theorem 4 below requires functions $f(x)$ with *zero mean*, that is, $\langle f\rangle = 0$. We note that $\langle\mathbf{a}\rangle = 0$ due to time reversibility and phase space volume conservation. We define a new function $\Delta T(x) = T(x) - \langle T\rangle$ so that $\langle\Delta T\rangle = 0$. This gives the fluctuations in the collision time about its average. Writing $T = \langle T\rangle + \Delta T$ in Eq. (5), removing the $\langle T\rangle$ term from the average, and taking the logarithm, we find

$$s(\mathbf{k}) = \lim_{n\to\infty} \frac{1}{2n\langle T\rangle} \ln\langle\exp[F(\mathbf{k})]\rangle \tag{6}$$

where

$$F(\mathbf{k})=\sum_{i=-n}^{n-1} f(\mathbf{k})\circ\boldsymbol{\phi}^i=\sum_{i=-n}^{n-1}[s(\mathbf{k})\Delta T\circ\boldsymbol{\phi}^i+\mathrm{i}\mathbf{k}\cdot\mathbf{a}\circ\boldsymbol{\phi}^i] \tag{7}$$

is a power series in $\mathbf{k}$ such that all the coefficients have zero mean.

Now we put the expression in the form of a cumulant expansion, which allows cancellation between similar terms of opposite sign, thus permitting the proof of convergence in Sec. 3. Expanding the exponential and the logarithm, and noting that $\langle F\rangle=0$ we find

$$s(\mathbf{k})=\lim_{n\to\infty}\frac{1}{2n\langle T\rangle}\sum_{N=2}^{\infty}Q_N(\mathbf{k}) \tag{8}$$

where the *cumulants* $Q_N(\mathbf{k})$ are defined by

$$Q_N(\mathbf{k})=\sum_{\{n_j\}:\sum_j jn_j=N}(-1)^{\nu-1}\frac{(\nu-1)!\prod_j\langle F^j\rangle^{n_j}}{\prod_j(n_j!j!^{n_j})} \tag{9}$$

with j and n_j integers satisfying $j\geq 2$ and $n_j\geq 0$, and $\nu=\sum_j n_j$ is the total number of correlations in the product. For example

$$\begin{aligned}
Q_2(\mathbf{k}) &= \langle F^2\rangle/2 && (10)\\
Q_3(\mathbf{k}) &= \langle F^3\rangle/6 && (11)\\
Q_4(\mathbf{k}) &= (\langle F^4\rangle-3\langle F^2\rangle^2)/24 && (12)\\
Q_5(\mathbf{k}) &= (\langle F^5\rangle-10\langle F^3\rangle\langle F^2\rangle)/120 && (13)\\
Q_6(\mathbf{k}) &= (\langle F^6\rangle-15\langle F^4\rangle\langle F^2\rangle-10\langle F^3\rangle^2+30\langle F^2\rangle^3)/720 && (14)
\end{aligned}$$

Using the definition of F, we can expand each cumulant as a power series in $\mathbf{k}$,

$$Q_N(\mathbf{k})=\sum_{m=N}^{\infty}q_{N,m;\alpha_1\ldots\alpha_m}k_{\alpha_1}\ldots k_{\alpha_m} \tag{15}$$

Note that to fixed order $\mathbf{k}^m$, only Q_N with $N\leq m$ appear, thus the rearrangement of the expansion from (6) to (8) involves only a finite number of terms, so questions of absolute convergence do not appear. This is the reason for the interpretation of these expressions as formal power series in $\mathbf{k}$ as indicated in the statement of Thm. 1. In Sec. 4 we ask whether such series converge for finite values of $\mathbf{k}$; it is apparent from Sec. 3 that convergence of the individual cumulants depends to a large extent on cancellations, so it is likely that Eq. (8) rather than Eq. (6) gives more consistent results at finite $\mathbf{k}$.

Writing Eq. (8) as a formal power series in $\mathbf{k}$ leads to an infinite set of (finite) equations for the unknowns $D^{(m)}$:

$$\mathrm{i}^m D^{(m)}_{\alpha_1\ldots\alpha_m}=\lim_{n\to\infty}\frac{1}{2n\langle T\rangle}\sum_{N=2}^{m}q_{N,m;\alpha_1\ldots\alpha_m} \tag{16}$$

Note that the $q_{N,m}$ contain $D^{(j)}$ with $j \leq m/2$ through the ΔT term in (7); thus we have an explicit equation for $D^{(m)}$, order by order, if the $n \to \infty$ limit in (8) converges.

Time reversal invariance and phase space volume conservation lead to equal and opposite contributions from correlations with odd powers of $\mathbf{a}$. Since each $\mathbf{a}$ corresponds to a single power of $\mathbf{k}$ and each ΔT corresponds to powers $m \geq 2$ at which $D^{(m)}$ is nonzero, we find that the terms $\langle a_\alpha a_\beta a_\gamma \rangle$ and $\langle \Delta T a_\alpha \rangle$ contributing to $D^{(3)}$ both vanish. The vanishing of $D^{(m)}$ for all odd m then follows by induction. Note that odd cumulants do not vanish, for example Q_3 contains the term $\langle \Delta T a_\alpha a_\beta \rangle$ which does not vanish, and contributes to $D^{(4)}$.

We remark that we have not yet used any information about the decay of correlations of the Lorentz gas, so the above expressions are valid for the Burnett coefficients of more general diffusive processes, as long as the $n \to \infty$ limit converges. For systems with a decay of correlations that is a (not too small) negative power of the time, we expect the first few Burnett coefficients to exist, see for example Ref. [10].

3 Convergence of the series

The averages $\langle F^{n_j} \rangle$ appearing in the cumulants contain summations over m variables with range $-n$ to $n-1$, and could grow as fast as $O(n^{n_j})$ in general. Thus each term, which is a product of such averages could grow as $O(n^N)$ in general. For the limit in Eq. (8) to exist, we require that the RHS grows only as $O(n)$. Although the growth of each product of correlations cannot be controlled this well, the following theorem is sufficient to imply the existence of the Burnett coefficients:

Theorem 3 *$q_{N,m}$ is defined in Eqs. (7, 9, 15) for integers N and m satisfying $2 \leq N \leq m$. $q_{N,m;\alpha_1 \ldots \alpha_m} = O(n)$ for all such N and m in the periodic Lorentz gas.*

To prove Thm. 3, we make use of the properties ("stretched exponential decay") of multiple correlations in the periodic Lorentz gas:

Theorem 4 *(Theorem 2 of Ref. [5]) Let $i_1 \leq \cdots \leq i_k$ and $1 \leq t \leq k-1$. Then*

$$|\langle f_1^{i_1} \cdots f_k^{i_k} \rangle - \langle f_1^{i_1} \cdots f_t^{i_t} \rangle \langle f_{t+1}^{i_{t+1}} \cdots f_k^{i_k} \rangle| \leq C_k \cdot |i_k - i_1|^2 \lambda^{|i_{t+1} - i_t|^{1/2}} \tag{17}$$

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

Here (and subsequently) f_j are piecewise Hölder continuous functions such that $\langle f_j \rangle = 0$ for all j. We put $f_j^i = f_j \circ \boldsymbol{\phi}^i$. In our case the f_j are ΔT or a_α. As noted in Ref. [5], we expect based on Refs. [11, 4] that it should be possible to prove a stronger bound $\lambda^{|i_{t+1} - i_t|}$, but the above bound is sufficient for our purposes here.

The $q_{N,m}$ as defined in the previous section are finite sums of terms of the form (see Eqs. (7, 9, 15))

$$\sum_{\{n_j\}:\sum_j jn_j=N} (-1)^{\nu-1}\frac{(\nu-1)!}{\prod_j(n_j!j!^{n_j})}\sum_{i_1\ldots i_N=-n}^{n-1}\langle f_1^{i_1}\ldots f_j^{i_j}\rangle\langle f_{j+1}^{i_{j+1}}\ldots\rangle\ldots\langle\ldots f_N^{i_N}\rangle \tag{18}$$

multiplied by constants such as the lower order Burnett coefficients.

In order to use Thm. 4 we need to put the times i_p in numerical order. It does not matter in which order the f_j are multiplied within a correlation, or which order correlations of equal numbers of f_j are multiplied; thus both factorials in the denominator disappear, leading to

$$\sum_{\{n_j\}:\sum_j jn_j=N} (-1)^{\nu-1}(\nu-1)!\Bigg[\sum_{i_1\leq i_2\ldots i_N}\frac{1}{S[i]}\langle f_1^{i_1}\ldots f_j^{i_j}\rangle\langle f_{j+1}^{i_{j+1}}\ldots\rangle\ldots\langle\ldots f_N^{i_N}\rangle \\ + \text{ permutations}\Big] \tag{19}$$

Here $S[i]$ is a combinatoric factor which takes account of the symmetry when some of the i_p are equal; the exact form is irrelevant because it does not depend on the n_j and so appears as a common prefactor. Equal times do not play a direct role in the application of Thm. 4, since we use the *largest* difference between the times $i_{t+1}-i_t$.

As an example, we give the expression for $N=6$:

$$\begin{aligned}\sum_{i_1\leq i_2\leq i_3\leq i_4\leq i_5\leq i_6} \quad & \frac{1}{S[i]}\Big\{\langle f_1^{i_1}f_2^{i_2}f_3^{i_3}f_4^{i_4}f_5^{i_5}f_6^{i_6}\rangle-\Big[\langle f_1^{i_1}f_2^{i_2}\rangle\langle f_3^{i_3}f_4^{i_4}f_5^{i_5}f_6^{i_6}\rangle+14\text{ permutations}\Big] \\ & -\Big[\langle f_1^{i_1}f_2^{i_2}f_3^{i_3}\rangle\langle f_4^{i_4}f_5^{i_5}f_6^{i_6}\rangle+9\text{ permutations}\Big] \\ & +2\Big[\langle f_1^{i_1}f_2^{i_2}\rangle\langle f_3^{i_3}f_4^{i_4}\rangle\langle f_5^{i_5}f_6^{i_6}\rangle+14\text{ permutations}\Big]\Big\}\end{aligned} \tag{20}$$

Now we apply Thm. 4 to the largest gap, $i_{t+1}-i_t$. Notice in the $N=6$ example, whatever the value of t, the theorem combines all the above correlations to leave a term bounded by $\lambda^{|i_{t+1}-i_t|^{1/2}}$ multiplied by powers of the time differences. Explicitly, for $t=1$, all terms cancel individually because $\langle f_j\rangle=0$. For $t=2$ the $\langle f^6\rangle$ term cancels with one of the $\langle f^2\rangle\langle f^4\rangle$ terms, six other $\langle f^2\rangle\langle f^4\rangle$ terms cancel with three of the $\langle f^2\rangle^3$ terms and the remaining terms all split leaving a $\langle f\rangle$ term. For $t=3$ the $\langle f^6\rangle$ term cancels with one of the $\langle f^3\rangle^2$ terms, and all of the others split leaving a $\langle f\rangle$ term. $t=4$ is analogous to $t=2$ and $t=5$ is analogous to $t=1$.

In general we must show that the coefficient $(-1)^{\nu-1}(\nu-1)!$ leads to complete cancellation for all values of N. Consider a general term (ignoring the $S[i]$ which is the same for each term) which is unaffected by a split at time t:

$$\langle\rangle\langle\rangle\ldots\langle\rangle|\langle\rangle\langle\rangle\ldots\langle\rangle \tag{21}$$

where all times i_p to the left of the bar "|" are less than or equal to t and all times to the right of the bar are greater than t. There are A correlations to the left and B correlations to the right, so $A+B=\nu$.

This term will cancel with any term which is split to the same form, that is, a term consisting of correlations that are either the same as the above, or combine one correlation from the left and one from the right. For example, when $N = 8$, a split at $t = 4$ combines $-6\langle f_1^{i_1} f_2^{i_2}\rangle\langle f_3^{i_3} f_4^{i_4}\rangle|\langle f_5^{i_5} f_6^{i_6}\rangle\langle f_7^{i_7} f_8^{i_8}\rangle$ with $2\langle f_1^{i_1} f_2^{i_2} f_5^{i_5} f_6^{i_6}\rangle\langle f_3^{i_3} f_4^{i_4}\rangle\langle f_7^{i_7} f_8^{i_8}\rangle$, $2\langle f_1^{i_1} f_2^{i_2} f_7^{i_7} f_8^{i_8}\rangle\langle f_3^{i_3} f_4^{i_4}\rangle\langle f_5^{i_5} f_6^{i_6}\rangle$, $2\langle f_1^{i_1} f_2^{i_2}\rangle\langle f_3^{i_3} f_4^{i_4} f_5^{i_5} f_6^{i_6}\rangle\langle f_7^{i_7} f_8^{i_8}\rangle$, $2\langle f_1^{i_1} f_2^{i_2}\rangle\langle f_3^{i_3} f_4^{i_4} f_7^{i_7} f_8^{i_8}\rangle\langle f_5^{i_5} f_6^{i_6}\rangle$, $-\langle f_1^{i_1} f_2^{i_2} f_5^{i_5} f_6^{i_6}\rangle\langle f_3^{i_3} f_4^{i_4} f_7^{i_7} f_8^{i_8}\rangle$ and $-\langle f_1^{i_1} f_2^{i_2} f_7^{i_7} f_8^{i_8}\rangle\langle f_3^{i_3} f_4^{i_4} f_5^{i_5} f_6^{i_6}\rangle$. These all cancel because $-6 + 2 + 2 + 2 + 2 - 1 - 1 = 0$.

The term given in Eq. (21) has coefficient $(-1)^{\nu-1}(\nu-1)!$. There are AB terms with coefficient $(-1)^{\nu-2}(\nu-2)!$ obtained by combining a single correlation on the left and the right. There are $A(A-1)B(B-1)/2!$ terms with coefficient $(-1)^{\nu-3}(\nu-3)!$ obtained by combining two correlations on the left and the right, and so on. The total coefficient is thus given by

$$\sum_{p=0}^{min(A,B)} (-1)^{A+B-p-1}(A+B-p-1)!\frac{A!B!}{(A-p)!(B-p)!p!} \tag{22}$$

To show that the coefficients cancel, we therefore need the following lemma:

Lemma 5 *The sum given by Eq. (22) is zero for all positive integers A and B.*

Proof: The sum is symmetric in A and B so suppose that $A \geq B$. Then the summand is the product of a constant $(-1)^{A+B-1}A!$, an alternating binomial of degree B, that is, $(-1)^{-p}B!/((B-p)!p!)$ and a polynomial in p of degree $B-1$, that is, $(A+B-p-1)!/(A-p)!$. Repeatedly summing by parts reduces the degree of both the alternating binomial and the polynomial until the result is zero, thus proving the lemma.

Given that all the correlations in the cumulants cancel leaving terms bounded by $\lambda^{|i_{t+1}-i_t|^{1/2}}$ times a polynomial in the time differences, the only terms making an appreciable contribution to the sum (19) are those with no sizable gap, that is, with all the times i_p close to each other. There are $O(n)$ of such terms, so Thm. 3 is proved. Eq. (16) gives the Burnett coefficients in terms of a finite number of the $q_{N,m}$ and so Thm. 1 is also proved.

4 Convergence of the Burnett expansion

Having established the existence of the Burnett coefficients $D^{(m)}$, we make a few remarks about the question of whether the expansion Eq. (4) converges for finite $\mathbf{k}$, Conj. 2. It is generally very difficult to estimate convergence numerically, because the many cancellations appearing in the cumulant expansion make an accurate computation beyond $m = 4$ very difficult, see for example Ref. [6].

There are two known results that make a finite radius of convergence for the Lorentz gas plausible. The first is that in the Boltzmann limit of a hard sphere gas, that is, a gas with many moving particles at low density and with recollisions ignored, the expansion in

$\mathbf{k}$ (in this context called the linearized Chapman-Enskog expansion) converges, Ref. [8]. Of course, the hard sphere collisions are similar to that of the Lorentz gas, but recollisions cannot be ignored in general.

The second result is exact, but for a highly simplified (piecewise linear) system. We consider the map

$$\phi(x) = \frac{3}{2} - 2x + 3[x] \tag{23}$$

which is equivalent to a random walk where the particle moves with equal probability from one interval $I_n = (n - 1/2, n + 1/2]$ to the left, I_{n-1} or to the right, I_{n+1}. The dispersion relation $s(k)$ follows directly from the solution, Eq. (3),

$$\rho(n,t) = \exp(st + ikn) \tag{24}$$

After one iteration,

$$\begin{aligned} \rho(n,1) &= \frac{1}{2}[\exp(\mathrm{i}k(n-1)) + \exp(\mathrm{i}k(n+1))] && (25) \\ &= \cos k \exp(\mathrm{i}kn) && (26) \end{aligned}$$

leading to

$$s(k) = \ln \cos k \tag{27}$$

which has a power series around $k = 0$ with a radius of convergence equal to $\pi/2$.

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