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Heat Conduction in Caricature Models of the Lorentz Gas

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Heat transport coefficients are calculated for various random walks with internal states (the Markov partition of the Sinai billiard connects these walks with the Lorentz gas among a periodic configuration of scatterers). Models with reflecting or absorbing barriers and also those without or with local thermal equilibrium are investigated. The method is unified and is based on the Keldysh expansion of the resolvent of a matrix polynomial.

KEY WORDS: Transport; Fourier law; random walks with internal states.

1. INTRODUCTION

The problem of heat conduction has inspired many fundamental ideas in mathematical physics. The deterministic heat equation was studied by Fourier as early as 1807 and his investigations were summed up in his famous book.[3] Since heat conduction is only one example of transport processes (e.g., neutron transport, electron scattering by impurities in a solid, etc.), it is impossible to survey even the most important developments of the theory. Nonetheless, "such well established experimental facts as Fourier's law of heat conduction or Fick's law of diffusion can neither be derived rigorously for general systems nor shown to hold for realistic microscopic models."[10] The explanation of this statement is that the theory of large systems of interacting particles, e.g., of those of hard balls interacting via elastic collisions, is moving forward only slowly. As a consequence, interest has turned to simplified, but far from simple, models, such as the Lorentz gas or the harmonic crystal.

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An intuitive description of the problem is the following: Consider a Lorentz gas in $\mathbb{R}^\nu$ with a $\mathbb{Z}^\nu$-periodic configuration of scatterers (for simplicity, we suppose they are spheres). We restrict the model to the strip between two barriers put at $x_1 = 0$ and $x_1 = L$ (L is a large integer) and serving as heat reservoirs kept at constant temperatures T_1 and T_2 ($> T_1$). A gas of noninteracting point particles is given in the strip. The motion of a single particle is uniform, with elastic collisions at the scatterers and with stochastic boundary conditions at the barriers: if a particle hits the wall $x_1 = 0$ ($x_1 = L$), it gets a new velocity independent of its incoming phase, with density equal to $\text{const} \times \exp[-(1/k_B T_1)(v, v)]$ for $v_1 > 0$ and to 0 for $v_1 \leqslant 0$ {to $\text{const} \times \exp[-(1/k_B T_2)(v, v)]$ for $v_1 < 0$ and to 0 for $v_1 \geqslant 0$, respectively}. In fact, the main requirements on the distributions of the outgoing velocities are that they are smooth and their second moments are proportional to the temperatures of the walls.

Now, from Goldstein *et al.*,[4] the existence of a steady state measure follows at any given density D of the gas particles and it also makes sense to define $E_{\text{tr}}(T_1, T_2, D, L)$ as the amount of energy transferred by the system between the two reservoirs per unit time and surface volume. Then the conductivity of the medium is defined as the thermodynamic limit

$$\kappa(T_1, T_2, D) = \lim_{L \to \infty} L E_{\text{tr}}(T_1, T_2, D, L) \tag{1.1}$$

and finally its heat conductivity coefficient at temperature T is

$$\kappa(T, D) = \lim_{\Delta t \to 0} (\Delta T)^{-1} \kappa(T_1, T_2, D) \tag{1.2}$$

where $T_1 = T - \frac{1}{2}\Delta T$ and $T_2 = T + \frac{1}{2}\Delta T$, provided that the limits (1.1) and (1.2) exist.

The aim of the present paper is to show the existence of $\kappa(T, D)$ and calculate its value for a caricature model of the Lorentz gas, namely for random walks with internal states (RWwIS). Now, (i) because of the periodicity of the scatterers, the dynamics of the Lorentz particle can be reduced to a Sinai billiard,[1] and (ii) the Markov partition of the Sinai billiard enables us to approximate it by a sequence of RWwIS's,[8] so the RWwIS's are legitimate models of the Lorentz dynamics and the strategy is justified that by handling the difficulties of the limit transition in their spectra, one also can obtain the corresponding results for the Lorentz gas. (We remark that, in the approximation, the internal states of the random walk correspond to elements of the Markov partition.)

The starting point of our investigation is the fundamental work of Lebowitz and Spohn,[11] where Fourier's law of heat conduction was derived in a different setup by also using an approximation via the linear

Boltzmann equation. The main differences are that their paper (i) considers stochastic scatterer configurations rather than deterministic ones, (ii) takes the Boltzmann–Grad limit with the mean free path tending to a positive constant, and (iii) only shows the existence of the heat conductivity coefficient defined by limits taken in reversed order:

$$\kappa_{\mathrm{LS}}(T, D) = \lim_{L \to \infty} L \lim_{\Delta t \to 0} (\Delta T)^{-1} E_{\mathrm{tr}}(T_1, T_2, D, L) \tag{1.3}$$

The calculation of the transport coefficients uses the tools of our technical papers[7,9] based on the Keldysh expansion of the resolvent of a matrix polynomial. In Section 2 we introduce our model: a continuous-time two-color RWwIS (with the colors representing the energy of the particle). The computation of κ then reduces to the asymptotic evaluation of the time-invariant distribution of this random walk (we remark that in Ref. 2 classical random walks were used to model heat conduction). Our main result says that

$$E_{\mathrm{tr}} = D\lambda \frac{(T_2 - T_1)(T_1 T_2)^{1/2}}{\sqrt{T_1} + \sqrt{T_2}} \sigma^2 + O(L^{-1})$$

where D is the density, λ is the proportionality constant in the jumping rates, and σ^2 is the variance of the RWwIS.

The generality of our method allows us to describe transport in various models. Thus, in Section 3, we treat heat transport in the sense of a simplified model suggested by Lebowitz and Spohn.[12] Here, both walls are absorbing and input only appears at one of them with a prescribed distribution among the internal states. Then the calculation of the transport coefficients is obtained from the asymptotic form of the solution of the Dirichlet problem.

Since the dynamics assumed in Section 2 does not involve local thermal equilibrium, one can only use a naive notion of temperature (=energy density per particle) to find its profile, which turns out to be linear fractional rather than linear. Therefore, in Section 4, we modify the model. We suppose that every lattice site has a local, *a priori* temperature derived from principles of zero particle flux and constant energy flux and from the given boundary temperatures T_1 and T_2. The local jumping rates of the RWwIS are determined by these local temperatures. In this less microscopic but more physical model the energy flux becomes

$$E_{\mathrm{tr}} = \tfrac{1}{4} D\lambda (T_2 - T_1)(\sqrt{T_1} + \sqrt{T_2}) + O(L^{-1})$$

and the temperature profile will be asymptotically linear. (We remark that

heat transport in a slightly analogous modification of a disordered harmonic chain has been studied by Rich and Visscher.[13]

Section 5 contains conclusions and remarks.

2. A TWO-COLOR RANDOM WALK WITH INTERNAL STATES (TCRWwIS): HEAT CONDUCTION WITHOUT LOCAL THERMAL EQUILIBRIUM

In our previous papers[7,8] we worked out the theory of discrete-time parameter random walks with internal states. For our purposes we need to extend the results of Ref. 7 to a slightly more complicated model with continuous-time parameter: to derive results directly applicable to the theory of heat conduction, we have to determine the stationary probabilities for a TCRWwIS to be defined below. The mathematical machinery of the computations—the spectral theory of matrix polynomials—is the same as in the aforementioned papers.

In order to explain the minor modifications needed for the TCRWwIS, we shall demonstrate the methods on the simplest nontrivial case. For treating the general case it is enough to repeat the corresponding proofs of Ref. 7. Let us turn to the definition of the TCRWwIS.

Definition 2.1. Let $\mathscr{E} = \{1,..., d\}$ be a finite set. A continuous-time parameter Markov process defined on the state space $\mathbb{Z} \otimes \mathscr{E} \otimes \{b, r\}$ (b: blue, r: red) as follows is called a TCRWwIS. Let us introduce the probability vectors

$$b(t, x) := (b_1(t, x),..., b_d(t, x))$$
$$r(t, x) := (r_1(t, x),..., r_d(t, x))$$

which give the probabilities

$$P(\xi_t = (x, k, b)) = b_k(t, x)$$
$$P(\xi_t = (x, k, r)) = r_k(t, x)$$

respectively; $x \in \mathbb{Z}$, $k \in \mathscr{E}$. We first give the forward Kolmogorov equations for $b(t, x)$ and $r(t, x)$:

$$\begin{aligned} \frac{\partial b(t, x)}{\partial t} &= \lambda_b[-b(t, x) + A^*_- b(t, x+1) + A^*_+ b(t, x-1)] \\ \frac{\partial r(t, x)}{\partial t} &= \lambda_r[-r(t, x) + A^*_- r(t, x+1) + A^*_- r(t, x-1)] \end{aligned} \tag{2.1}$$

Here A_+ and A_- are nonnegative $d \times d$ matrices such that $A_+ + A_- = Q$ is a stochastic matrix and $\lambda_b < \lambda_r$ are two positive constants, namely the jumping rates for $\xi_t = (\cdot, \cdot, b)$ and $\xi_t = (\cdot, \cdot, r)$, respectively. The transitions of ξ_t from a state of the type $(\cdot, \cdot, b)$ to a state of the type $(\cdot, \cdot, r)$ and vice versa take place through the exchange rules at the boundaries $x = 0$ and $x = L$ after restricting the phase space $\mathbb{Z} \otimes \mathscr{E} \otimes \{b, r\}$ to $\{0, 1, ..., L\} \otimes \mathscr{E} \otimes \{b, r\}$.

An intuitive description of this process is the following: the walking particle has an internal state and a color. When hitting the wall at 0 (at L) the color becomes blue (red). The jumping rate only depends on the color, namely it is λ_b or λ_r. The particle only jumps to nearest neighbor lattice sites and the probability for the transition of internal states is given by the matrix A_- or A_+ if the jump is -1 or $+1$, respectively. If in 0 or 1 the above rule resulted in a jump to the left, then the new site of the particle will be 0 (the blue boundary), its color becomes (or remains) blue, and by definition the particle changes its internal states after the jump again, according to the stochastic matrix S_1. This matrix S_1 expresses the effect of the wall (or heat reservoir) on the internal states. Analogous statements hold for the other wall (the site L) with another stochastic matrix S_2. In order to avoid cumbersome formulas, we assume that each row of the matrix S_1 (S_2) is equal to the vector π_1 (π_2).

Now we briefly repeat the conditions imposed on A_+ and A_- in Ref. 7.

Set $A_+ := (a_{ij}^+)$ and $A_- := (a_{ij}^-)$.

(i) $Q = A_+ + A_-$ is an ergodic, aperiodic stochastic matrix, so there exists a unique stationary probability vector $\mu = (\mu_1, ..., \mu_d)^*$ such that

(ii) $\mu_i a_{ij}^+ = \mu_j a_{ji}^-$ (reversibility)

(iii) For every $j, k \in \mathscr{E}$ and $m \in \mathbb{Z}$ there exists a natural number n and a sequence $\{\delta_1, ..., \delta_n\}$ of plus and minus signs such that $(\prod_{s=1}^n A_{\delta_s})_{j,k} > 0$ and the number of plus signs in $\{\delta_1, ..., \delta_n\}$ is equal to $(m+n)/2$.

Set

$$\mathbb{1} := \underbrace{(1, ..., 1)^*}_{d \text{ times}}$$

Conditions (i)–(iii) imply the centralization condition

$$((A_+ - A_-)\mathbb{1}, \mu) = 0 \tag{2.2}$$

and the nondegeneracy condition: for every representive e of

$(I-Q)^{-1}(A_+ - A_-)\mathbb{1}$ [which exists by virtue of (2.2)] $1 + 2((A_+ - A_-)e, \mu) := \sigma^2 > 0$ (for proofs see Ref. 7).

Throughout this paper, we assume for simplicity that A_+ (and consequently A_-) is invertible. The equations for the stationary probability vectors $b(x)$ and $r(x)$ derived from the forward Kolmogorov equations are

$$\begin{aligned} b(x) &= A_+^* b(x-1) + A_-^* b(x+1) \\ r(x) &= A_+^* r(x-1) + A_-^* r(x+1) \end{aligned} \qquad (0 < x < L) \tag{2.3}$$

$$\begin{aligned} \lambda_b b(0) &= S_1^* A_-^* [\lambda_b b(0) + \lambda_b b(1) + \lambda_r r(1)] \\ \lambda_r r(L) &= S_2^* A_+^* [\lambda_r r(L) + \lambda_r r(L-1) + \lambda_b b(L-1)] \\ r(0) &= 0 \\ b(L) &= 0 \end{aligned} \tag{2.4}$$

The boundary conditions (2.4) describe the exchange rules $(\cdot, \cdot, b) \rightleftarrows (\cdot, \cdot, r)$. We are looking for $b(x)$ and $r(x)$ in the form of linear combinations of d-dimensional, vector-valued functions

$$\rho^x f_s + \binom{x}{1} \rho^{x-1} f_{s-1} + \cdots + \binom{x}{s} \rho^{x-s} f_0$$

Here f_0 is the eigenvector of the matrix polynomial $S(\rho) := A_-^* \rho^2 - I\rho + A_+^*$ (I is the $d \times d$ identity matrix) corresponding to the eigenvalue ρ [$\det S(\rho) = 0$], while $f_1, \ldots, f_s$ are the cyclic vectors, if they exist. They are defined by the chain of equations

$$\begin{aligned} S(\rho) f_0 &= 0 \\ S(\rho) f_1 + \frac{1}{1!} \frac{\partial S(\rho)}{\partial \rho} f_0 &= 0 \\ &\vdots \\ S(\rho) f_s + \cdots + \frac{1}{s!} \frac{\partial^s S(\rho)}{\partial \rho^s} f_0 &= 0 \end{aligned}$$

All the properties of the matrix polynomial $S(\rho)$ needed for the solution of Eqs. (2.3) and (2.4) are formulated and proved in our previous papers. First we recall two of them, which essentially determine the structure of the solution:

Statement 2.1. 1 is the only eigenvalue of $S(\rho)$ on the unit circle. The corresponding eigenvector is μ. There exists exactly one cyclic vector $f_1 = (Q^* - I)^{-1}(A_+^* - A_-^*)\mu$ belonging to it.

Statement 2.2. The equation $\det S(\rho) = 0$ has exactly $d-1$ roots inside the unit circle. If ρ is a root, then $\bar{\rho}$ and ρ^{-1} are also roots with the same multiplicity and the same structure of cyclic vectors.

For the sake of brevity, we assume that there are no cyclic vectors. Let f_ρ denote the eigenvector corresponding to the root ρ. In order to get symmetry of the formulas near the boundaries $x=0$ and $x=L$, we seek the stationary probabilities in the following form:

$$\begin{aligned}\lambda_b b(x) &= \varphi_0^b \mu + \varphi_1^b[(L-x)\mu - f_1] + \sum_{|\rho|<1} \varphi_\rho^b \rho^x f_\rho + \sum_{|\rho|>1} \varphi_\rho^b \rho^{x-L} f_\rho \\ \lambda_r r(x) &= \varphi_0^r \mu + \varphi_1^r(x\mu + f_1) + \sum_{|\rho|<1} \varphi_\rho^r \rho^x f_\rho + \sum_{|\rho|>1} \varphi_\rho^r \rho^{x-L} f_\rho\end{aligned} \tag{2.5}$$

where the unknown coefficients $\varphi_0^b, \varphi_1^b, \ldots, \varphi_\rho^b, \ldots, \varphi_0^r, \ldots, \varphi_\rho^r, \ldots$ are to be determined from the boundary conditions (2.4) and from the normalizing condition

$$\sum_{x=0}^{L} (b(x) + r(x), \mathbb{1}) = 1 \tag{2.6}$$

Note. The Keldysh method on the resolvent of matrix polynomials implies the independence of the vector system $\{\mu; f_\rho: |\rho|<1\}$ and of the system $\{\mu; f_\rho: |\rho|>1\}$ (cf. Proposition 4.4 in Ref. 9). This implies that each solution of (2.3) can be written in the form of (2.5) with uniquely determined coefficients $\varphi_0^b, \varphi_1^b, \ldots$. For our further computation it will be convenient to write Eqs. (2.4) in the following order: third, first, fourth, and second:

$$\begin{aligned}&\varphi_0^b \begin{pmatrix} 0 \\ \pi_1 - \mu \\ \mu \\ \pi_2 \end{pmatrix} + \varphi_1^b \begin{pmatrix} 0 \\ S_1^* A_-^* [(2L-1)\mu - 2f_1] - L\mu + f_1 \\ -f_1 \\ S_2^* A_+^* (\mu - 2f_1) \end{pmatrix} \\ &+ \sum_{|\rho|<1} \varphi_\rho^b \begin{pmatrix} 0 \\ (f_\rho, \mathbb{1})\pi_1 - f_\rho \\ O(\kappa^L) \\ O(\kappa^L) \end{pmatrix} + \sum_{|\rho|>1} \varphi_\rho^b \begin{pmatrix} 0 \\ O(\kappa^L) \\ f_\rho \\ (f_\rho, \mathbb{1})\pi_2 \end{pmatrix} \\ &+ \varphi_0^r \begin{pmatrix} \mu \\ \pi_1 \\ 0 \\ \pi_2 - \mu \end{pmatrix} + \varphi_1^r \begin{pmatrix} f_1 \\ S_1^* A_-^* (\mu + 2f_1) \\ 0 \\ S_2^* A_+^* [(2L-1)\mu + 2f_1] - L \end{pmatrix} \\ &+ \sum_{|\rho|<1} \varphi_\rho^r \begin{pmatrix} f_\rho \\ (f_\rho, \mathbb{1})\pi_1 \\ 0 \\ O(\kappa^L) \end{pmatrix} + \sum_{|\rho|>1} \varphi_\rho^r \begin{pmatrix} O(\kappa^L) \\ O(\kappa^L) \\ 0 \\ (f, \mathbb{1})\pi_2 - f_\rho \end{pmatrix} = 0\end{aligned} \tag{2.7}$$

This is a homogeneous system of $4d$ linear equations for the $4d$ variables $\varphi_0^b, \varphi_1^b, \ldots$. It turns out that the rank of the matrix of this system is equal to $4d-1$ and the condition (2.6) will guarantee the uniqueness of the solution, as in Ref. 7. We note that κ is a fixed constant, such that $\max_{|\rho|<1}\{|\rho|\}<\kappa<1$. So the $O(\kappa^L)$ terms are exponentially small in the system of equations (2.7) and they can be omitted, giving an exponentially small error in the variables φ_0^b and consequently in the probabilities $r(x)$ and $b(x)$. To obtain (2.7) we used the identities

$$S_1^* A_-^* \mu = \pi_1, \qquad 2S_2^* A_+^* \mu = \pi_2$$

$$S_1^* A_-^* f_\rho = (A_-^* f_\rho, \mathbb{1})\,\pi_1 = (f_\rho, \mathbb{1})\pi_1/(\rho+1)$$

$$S_2^* A_+^* f_\rho = (A_+^* f_\rho, \mathbb{1})\,\pi_2 = \rho(f_\rho, \mathbb{1})\pi_2/(\rho+1)$$

which follow easily from the properties of S_1 and S_2 and from $Q\mathbb{1}=1$, $S(\rho)f_\rho = 0$.[7] Subtracting the sum of the first d equations from the sum of the second d equations and neglecting the exponential terms, one gets

$$[-\tfrac{1}{2} - 2(f_1, A_-\mathbb{1}) + (f_1, \mathbb{1})]\,\varphi_1^b + [\tfrac{1}{2} + 2(f_1, A_-\mathbb{1}) - (f_1, \mathbb{1})]\,\varphi_1^r = 0$$

The number $\frac{1}{2} + 2(f_1, A_-\mathbb{1}) - (f_1, \mathbb{1})$ is equal to $\sigma^2/2 \neq 0$, as we can easily see from the definitions. Thus, $\varphi_1^b = \varphi_1^r = \psi$. [We note that the equality $\varphi_1^b = \varphi_1^r$ is exact, because the neglected $O(\kappa^L)$ vectors are orthogonal to $\mathbb{1}$.]

Now we suppose the following natural conditions:

$$\pi_1 \notin \operatorname*{span}_{|\rho|<1}\{f_\rho\}, \qquad \pi_2 \notin \operatorname*{span}_{|\rho|>1}\{f_\rho\} \tag{2.8}$$

[for example, in the case $\pi_1 = \mu = \pi_2$, the conditions (2.8) are satisfied in virtue of Proposition 4.4 in Ref. 9]. Now (2.8) and the above-mentioned independence of eigenvectors imply that the vectors

$$\begin{pmatrix}\mu\\ \pi_1\end{pmatrix};\ \left\{\begin{pmatrix}0\\ (f_\rho, \mathbb{1})\,\pi_1 - f_\rho\end{pmatrix}\right\}_{|\rho|<1};\ \left\{\begin{pmatrix}f_\rho\\ (f_\rho, \mathbb{1})\,\pi_1\end{pmatrix}\right\}_{|\rho|<1} \tag{2.9}$$

and the vectors

$$\begin{pmatrix}\mu\\ \pi_2\end{pmatrix};\ \left\{\begin{pmatrix}0\\ (f_\rho, \mathbb{1})\,\pi_2 - f_\rho\end{pmatrix}\right\}_{|\rho|>1};\ \left\{\begin{pmatrix}f_\rho\\ (f_\rho, \mathbb{1})\,\pi_2\end{pmatrix}\right\}_{|\rho|>1} \tag{2.10}$$

form two bases in the orthogonal complement of the vector

$$\begin{pmatrix}-\mathbb{1}\\ \mathbb{1}\end{pmatrix}$$

Putting the terms with $\varphi_1^b = \varphi_1^r = \psi$ of (2.7) on the right hand side, then expressing the upper $(2d)$ size columns in terms of the base (2.9) and the lower ones in terms of the base (2.10), and finally eliminating some coefficients of φ_0^b and φ_0^r, we get the following solutions of (2.7):

$$\begin{aligned}
\varphi_0^b &= [\gamma_0 + O(\kappa^L)]\psi \\
\varphi_\rho^b &= [C_\rho L + \beta\rho + O(\kappa^L)]\psi \qquad (|\rho| < 1) \\
\varphi_\rho^b &= [\gamma_\rho + O(\kappa^L)]\psi \qquad (|\rho| > 1) \\
\varphi_0^r &= [\alpha_0 + O(\kappa^L)]\psi \\
\varphi_\rho^r &= [\alpha_\rho + O(\kappa^L)]\psi \qquad (|\rho| < 1) \\
\varphi_\rho^r &= [d_\rho L + \delta_\rho + O(\kappa^L)]\psi \qquad (|\rho| > 1)
\end{aligned} \tag{2.11}$$

where the constants α_0, γ_0, α_ρ, γ_ρ, etc., can be expressed with the help of the vectors $\mu, f_1, f_\rho, \pi_1, \pi_2$. The actual expressions of these constants are completely unnecessary; the only important fact will be the order of the numbers φ_0^b, φ_ρ^b, φ_0^r, φ_ρ^r compared with ψ, as we shall see soon.

Let us use the normalizing condition (2.6), giving physical meaning to the model investigated in this section.

Because of the infinity and the periodicity of the medium in $\nu - 1$ dimensions, our model is essentially one-dimensional. The process represents a particle moving between two boundaries $x = 0$ and $x = L$, which we assume to be heat reservoirs of temperatures T_1 and T_2, respectively (say $T_1 < T_2$). A particle in a state of the type $(\cdot, \cdot, b)$ or $(\cdot, \cdot, r)$ transports an amount of energy proportional to T_1 or T_2, respectively. Due to the physical meaning of the temperature (it is proportional to the mean square of the velocities of the particles), it is reasonable to assume that $\lambda_b \sim \sqrt{T_1}$ and $\lambda_r \sim \sqrt{T_2}$. Further, since, in general, one gets a central limit theorem if the space variable is normed by L and the time variable (λ^{-1}) is normed by L^2, the computations lead to correct results upon setting

$$\lambda_b = \lambda L^2 \sqrt{T_1}, \qquad \lambda_r = \lambda L^2 \sqrt{T_2} \tag{2.12}$$

(λ is a fixed proportionality constant). Now it is easy to derive from (2.6) with help of (2.5), (2.11), and (2.12) the expression for ψ:

$$\psi = \frac{2\lambda (T_1 T_2)^{1/2}}{\sqrt{T_1} + \sqrt{T_2}} + O(L^{-1}) \tag{2.13}$$

To determine the energy flux E_{tr} it is enough to compute the energy

exchange in the middle, say between the places x and $x+1$, where $x = [L/2]$, so

$$E_{\mathrm{tr}} = D[T_2((A_-^* \lambda_r r(x+1), \mathbb{1}) - (A_+^* \lambda_r r(x), \mathbb{1})) + T_1((A_-^* \lambda_b b(x+1), \mathbb{1}) - (A_+^* \lambda_b b(x), \mathbb{1}))]$$

(D is the density of the matter). Using (2.5), the approximation (2.11), the equality $\sigma^2 = 1 + 2(f_1, (A_- - A_+)\mathbb{1})$, and expression (2.13), we get

$$E_{\mathrm{tr}} = D(T_2 - T_1)\frac{\sigma^2}{2}\psi = D\lambda \frac{(T_2 - T_1)(T_1 T_2)^{1/2}}{\sqrt{T_1} + \sqrt{T_2}}\sigma^2 + O(L^{-1}) \quad (2.14)$$

The temperature profile corresponding to our model can be determined without any further assumption:

$$T_L(x) = \frac{\text{density of energy at } x}{\text{density of particle at } x}$$

Using (2.5), (2.11), and (2.12), we have

$$T_L(x) = \frac{T_1(\mathbb{1}, b(x)) + T_2(\mathbb{1}, r(x))}{(\mathbb{1}, b(x)) + (\mathbb{1}, r(x))} = \frac{T_1^{1/2}(L-x) + T_2^{1/2}x}{T_1^{-1/2}(L-x) + T_2^{-1/2}x} + O(L^{-1})$$

$$= \frac{T_2^{1/2}(x/L) + T_1^{1/2}(1-x/L)}{T_2^{-1/2}(x/L) + T_1^{-1/2}(1-x/L)} + O(L^{-1})$$

if

$$0 < \gamma_1 \leqslant x/L \leqslant \delta_1 < 1$$

3. TRANSPORT WITH PRESCRIBED INCOMING DENSITIES AT THE BOUNDARY

A simplified way to define a transport coefficient has been proposed in Ref. 12. We shall approximate the Lorentz process with the RWwIS as in Section 2. Now we do not deal with cold and warm particles, i.e., there is only one type of particle. For simplicity, we shall work with discrete-time parameters. Suppose that independent particles are walking randomly between the absorbing walls $x = 0$ and $x = L$. This RWwIS is directed by the matrices A_- and A_+. Moreover, in each moment of time some new particles appear at the site $x = L$ and in the internal state j ($j = 1, 2, \ldots, d$). The number of these new particles is a random variable ξ_j with non-negative integer values and with finite expectation π_j. By definition, these

new particles can only be absorbed at the absorbing wall $x = L$ at their next return. We can define the vectors $u(x)$ $(x = 0, 1, \ldots, L)$, where the jth component of $u(x)$ is the time-invariant expected value of the number of particles in the state (x, j). It is easy to see that these expected values are finite and, for the vectors $u(x)$, the following equations and boundary conditions hold:

$$u(x) = A_+^* u(x-1) + A_-^* u(x+1) \qquad (0 < x < L) \tag{3.1}$$

$$u(0) = 0; \qquad u(L) = \pi = (\pi_1, \ldots, \pi_d)^* \tag{3.2}$$

Denote by $j_L(D)$ the rate per unit time of particles being absorbed at the wall $x = 0$. [Hence D is the density of the incoming particles, i.e., $D = (\mathbb{1}, \pi) = \sum_j \pi_j$.] Then

$$\tilde{\kappa}(D) = \lim_{\substack{L \to \infty \\ L - x_L \to \infty}} \frac{L j_L(D)}{(u(x_L + 1) - u(x_L), \mathbb{1})}$$

is a temperature-independent version of a transport coefficient. (In this model the denominator can be regarded as the density gradient.) By definition, $j_L = (\mathbb{1}, A_-^* u(1))$. According to Ref. 7, the general solution of (3.1) is

$$u(x) = \varphi_0 \mu + \varphi_1 (x\mu + f_1) + \sum_{|\rho| < 1} \varphi_\rho \rho^x f_\rho + \sum_{|\rho| > 1} \varphi_\rho \rho^{x-L} f_\rho \tag{3.3}$$

The boundary conditions give the equations

$$\varphi_0 \mu + \varphi_1 f_1 + \sum_{|\rho| < 1} \varphi_\rho f_\rho = O(\kappa^L)$$

$$\varphi_0 \mu + \varphi_1 (L\mu + f_1) + \sum_{|\rho| > 1} \varphi_\rho f_\rho = \pi + O(\kappa^L)$$

Because of the conservation of the flux

$$j_L = (\mathbb{1}, A_-^* u(1)) = (\mathbb{1}, A_-^* u(x) - A_+^* u(x-1)) \qquad (0 < x < L)$$

If $x \sim L/2$, then, in (3.3), the main term in the asymptotics is the linear one and, following Ref. 9 (or Section 2 of this paper),

$$\lim_{L \to \infty} L j_L = \frac{\sigma^2}{2} \frac{\det(\pi; f_\rho : |\rho| < 1)}{\det(\mu; f_\rho : |\rho| < 1)} \tag{3.4}$$

Similarly

$$\lim_{\substack{L \to \infty \\ L - x_L \to \infty}} (u(x_L + 1) - u(x_L), \mathbb{1}) = \frac{\det(\pi; f_\rho : |\rho| < 1)}{\det(\mu; f_\rho : |\rho| < 1)}$$

The following phenomenon is surprising: In general,

$$\lim_{x \to 1} \lim_{L \to \infty} (u(x_L), \mathbb{1}) \neq D$$

and the equality holds if and only if one has the martingale situation of Remark 5.6 in Ref. 7.

4. HEAT CONDUCTION WITH LOCAL THERMAL EQUILIBRIUM

Now we assume that the grid points $1, 2, \ldots, L-1$ take part in the energy transport. Let ξ_t be a continuous-time parameter RWwIS on the phase space $\mathbb{Z} \otimes \mathscr{E}$, which represents a particle transporting the energy. The transition matrices A_+ and A_- are the same as in Section 2, but the jumping rate is a (deterministic) function $\lambda(x)$ of $x \in \{0, 1, \ldots, L\}$. It is natural to assume that $\lambda(x) = \lambda_L [T_L(x)]^{1/2}$, where $T_L(x)$ is the unknown steady-state temperature profile. Our aim is to derive the shape of $T_L(x)$ from the fact that in steady state the energy flux does not depend on x. The subscript L means that the phase space of ξ_t is $[0, L] \otimes \mathscr{E}$. We shall determine the limit temperature profile when $L \to \infty$ and finally, as in the preceding section, setting $\lambda_L = \lambda L^2$, compute the limit energy flux.

Let us recall the forward Kolmogorov equation for the stationary probability vector $p(x)$ of ξ_t: For $x \in [1, L-1]$

$$\lambda(x)\, p(x) = A_+^*\, \lambda(x-1)\, p(x-1) + A_-^*\, \lambda(x+1)\, p(x+1) \tag{4.1}$$

and for $x = 0$, $x = L$

$$\begin{aligned} \lambda(0)\, p(0) &= A_-^*\, \lambda(0)\, p(0) + A_-^*\, \lambda(1)\, p(1) \\ \lambda(L)\, p(L) &= A_+^*\, \lambda(L)\, p(L) + A_+^*\, \lambda(L-1)\, p(L-1) \end{aligned} \tag{4.2}$$

The energy flux between $x-1$ and x is equal to

$$E_{\mathrm{tr}} = D\lambda L^2 (\mathbb{1}, -T_L^{3/2}(x-1)\, A_+^*\, p(x-1) + T_L^{3/2}(x)\, A_-^*\, p(x)) \tag{4.3}$$

The absence of particle flux is the consequence of the stationarity:

$$(\mathbb{1}, [T_L(x-1)]^{1/2}\, A_+^*\, p(x-1) - [T_L(x)]^{1/2}\, A_-^*\, p(x)) = 0 \tag{4.4}$$

One gets from (4.3) and (4.4) that

$$E_{\mathrm{tr}} = D\lambda L^2 [-T_L(x-1) + T_L(x)](A_-\mathbb{1}, [T_L(x)]^{1/2}\, p(x)) \tag{4.5}$$

The main theorem of Ref. 7 gives exact asymptotics for $p(x)[T(x)]^{1/2}$ when $L \to \infty$:

$$p(x)[T(x)]^{1/2} = \frac{C_L}{L + a_0}[\mu + w_1(x) + v_1(L - x)] + O(\kappa^L)$$

where $0 < \kappa < 1$, $w_1(x) = O(\kappa^x)$, and $v_1(x) = O(\kappa^x)$. So

$$[T_L(x)]^{1/2} p(x) = \frac{C_L}{L + a_0}\mu + O(L^{-1}(\kappa^x + \kappa^{L-x})) \tag{4.6}$$

The substitution of (4.6) into (4.5) gives

$$T_L(x) - T_L(x-1) = \frac{2E_{\text{tr}}(L + a_0)}{D\lambda L^2 C_L(1 + O(\kappa^x + \kappa^{L-x}))} \tag{4.7}$$

Summing (4.7) over $x \in [1, L]$, we get

$$\begin{aligned} T_2 - T_1 &= \frac{2E_{\text{tr}}[1 + O(1/L)]}{D\lambda C_L} \sum_{x=1}^{L} \frac{1}{L[1 + O(\kappa^x + \kappa^{L-x})]} \\ &= \frac{2E_{\text{tr}}}{D\lambda C_L} + O\left(\frac{1}{L}\right) \end{aligned} \tag{4.8}$$

[observe that $\sum_{x=1}^{L} \{L[1 + O(\kappa^x + \kappa^{L-x})]\}^{-1} = 1 + O(1/L)$] and C_L and C_L^{-1} are bounded functions of L; this last statement is a consequence of the boundedness of $T_L(x)$ and of the fact that $p(x)$ is a probability distribution on $[0, L] \otimes \mathscr{E}$. So

$$\frac{E_{\text{tr}}}{D\lambda C_L} = \frac{T_2 - T_1}{2} + O\left(\frac{1}{L}\right) \tag{4.9}$$

Then (4.7) and (4.9) yield

$$\begin{aligned} T_L(k) - T_L(k-1) = [T_2 - T_1 + O(L^{-1})][1 + O(L^{-1}))] \\ + \frac{1}{L[1 + O(\kappa^k + \kappa^{L-k})]} \end{aligned} \tag{4.10}$$

Summing (4.10) over k from 1 to x,

$$T_L(x) - T_1 = \frac{T_2 - T_1 + O(L^{-1})}{L} \sum_{k=1}^{x} [1 + O(\kappa^k + \kappa^{L-k})]^{-1}$$

which means that the temperature profile is linear up to the order $O(L^{-1})$:

$$T_L(x) = T_1 + (T_2 - T_1)x/L + O(L^{-1}) \tag{4.11}$$

Finally, we shall determine the energy flux. To this end first we compute C_L. Formulas (4.6) and (4.11) give

$$p(x) = \left[T_1 + (T_2 - T_1)\frac{x}{L} + O(L^{-1}) \right]^{-1/2} \left[\frac{C_L}{L + a_0} \mu + O(L^{-1}(\kappa^x + \kappa^{L-x})) \right]$$

$$= \frac{C_L \mu}{L[T_1 + (T_2 - T_1)x/L]^{1/2}} + O(L^{-2}) + O(L^{-1}(\kappa^x + \kappa^{L-x}))$$

Since $p(x)$ is a probability distribution on $[0, L] \otimes \mathscr{E}$, $\sum_{x=0}^{L} (p(x), \mathbb{1}) = 1$. Consequently,

$$1 = C_L \sum_{x=0}^{L} \frac{L^{-1}}{[T_1 + (T_2 - T_1)x/L]^{1/2}} + O(L^{-1}) \tag{4.12}$$

The $\sum$ in the last formula is a Riemann approximation for the integral

$$\int_0^1 \frac{dy}{[T_1 + (T_2 - T_1)\, y]^{1/2}}$$

Computing this integral, (4.12) gives the asymptotics of C_L:

$$C_L = \frac{\sqrt{T_1} + \sqrt{T_2}}{2} + O(L^{-1})$$

Substituting this into (4.9), we get the asymptotics for the energy flux

$$E_{\text{tr}} = \tfrac{1}{4} D\lambda (T_2 - T_1)(\sqrt{T_1} + \sqrt{T_2}) + O(L^{-1})$$

5. CONCLUSIONS AND A REMARK

We have calculated the heat conductivity for various caricature models of the Lorentz gas with a periodic configuration of scatterers, namely:

(i) For random walks with internal states between two heat reservoirs kept at constant temperatures (T_1 and T_2) (a) in absence of thermal equilibrium (Section 2) and (b) with thermal equilibrium (Section 4).

(ii) For random walks with internal states between two absorbing barriers with a constant rate of incoming flux of particles at one of the walls (Section 3).

Through the method of Markov partitions these stochastic evolutions are natural approximations of the deterministic Lorentz dynamics. In these models the square of the jumping rate corresponds to the energy. While in

the models of type (i) it remains constant between the walls, in model (ii) it changes from point to point, corresponding to the local temperature determined by the conservation laws.

The following expressions are obtained for the conductivities:

Model (ia):

$$\kappa(T_1, T_2, D) = \sigma^2 D\lambda \frac{(T_2 - T_1)\, T_1^{1/2} T_2^{1/2}}{T_1^{1/2} + T_2^{1/2}} \tag{5.1}$$

Model (ib):

$$\kappa_{\tilde{\pi}}(D) = \tfrac{1}{2}\sigma^2 D\lambda$$

where

$$\kappa_{\tilde{\pi}}(D) = \tilde{\kappa}(D) \qquad \text{with} \quad D = (\mathbb{1}, \pi), \quad \tilde{\pi} = D^{-1}\pi \tag{5.2}$$

Model (ii):

$$\kappa(T_1, T_2, D) = \tfrac{1}{4} D\lambda (T_2 - T_1)(T_1^{1/2} + T_2^{1/2}) \tag{5.3}$$

Here $\tilde{\pi}$ is the internal state distribution of the incoming particles in model (ii); further, λ is a proportionality constant in the jumping rates, D is the particle density, and σ^2 is the diffusion coefficient of the RWwIS.

In expression (5.1), the dependence of the conductivity on the RWwIS (or on the geometry of the scatterer configuration of the Lorentz gas) is compressed in the factor σ^2.

The universality of (5.3), i.e., its independence of the RWwIS, may, at first glance, be surprising. Observe, however, that in model (ii) the energy exchange depends on the short-range $[O(1)]$ behavior of the RWwIS.

Observe that, though the dependence of $\kappa(T_1, T_2, D)$ on T_1 and T_2 is different in the models of Sections 2 and 4, the heat conductivity coefficients $\kappa(T, D)$ are of the same form, const $\times \sqrt{T}$.

Remark. An additional problem where our approach is applicable is that of transport in a composite medium. We mean a Lorentz gas (or a TCRWwIS) between two walls $x_1 = 0$ and $x_1 = 2L$ where the scatterers form a periodic configuration between $x_1 = 0$ and $x_1 = L$ and another periodic configuration between $x_1 = L$ and $x_1 = 2L$. The solution of the problem for the RWwIS leads to finding the asymptotics of the solution of a $4d \times 4d$ homogeneous system of equations [cf. (2.4)], while for the TCRWwIS the size is doubled $(8d \times 8d)$.

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