

## Exponential approach to, and properties of, a non-equilibrium steady state in a dilute gas

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*Dedicated to Errico Presutti, friend and mentor.*

**Abstract.** We investigate a kinetic model of a system in contact with several thermal reservoirs at different temperatures  $T_\alpha$ . Our system is a spatially uniform dilute gas whose internal dynamics is described by the non-linear Boltzmann equation with Maxwellian collisions. Similarly, the interaction with reservoir  $\alpha$  is represented by a Markovian process that has the Maxwellian  $M_{T_\alpha}$  as its stationary state. We prove existence and uniqueness of a non-equilibrium steady state (NESS) and show exponential convergence to this NESS in a metric on probability measures introduced into the study of Maxwellian collisions by Gabetta, Toscani and Wennberg (GTW). This shows that the GTW distance between the current velocity distribution to the steady-state velocity distribution is a Lyapunov functional for the system. We also derive expressions for the entropy production in the system plus the reservoirs which is always positive.

### 1 Introduction

The existence, uniqueness and nature of a non-equilibrium steady state (NESS) of a system in contact with several reservoirs at different temperatures and/or chemical potentials continues to be one of the central problems in statistical mechanics, as is the approach to such a state. There are only a few models in which the isolated system evolves according to classical Hamiltonian mechanics or according to quantum mechanics for which we have even partial answers to these questions (Bonetto et al. (2000), Dhar (2008), Lepri et al. (2003), Goldstein et al. (1978)). In addition to the rather unphysical models corresponding to harmonic crystals and ideal gases, existence and uniqueness was proven for systems interacting with soft potentials in contact with thermal walls (Kipnis et al. (1985)). The resulting NESS is spatially non-uniform, and we have little information about its structure. This is true to a large extent even for cases in which the system is described mesoscopically by a one particle distribution  $f(x, v, t)$ , as in kinetic theory, where correlations between particles are negligible. For information about this important case,

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*Key words and phrases.* Non-equilibrium steady state, Boltzmann equation.  
Received September 2014; accepted September 2014.

we refer the reader to [Eposito et al. \(1994\)](#), [Arkeryd and Nourri \(2000\)](#) and references in the latter paper’s extensive bibliography. Both papers consider diffuse boundary conditions at different temperatures, and existence of an NESS is the main result.

More is possible to prove for NESS of kinetic systems that are spatially uniform. Such a system, with one reservoir, but acted upon by an electric field, is investigated in [Carlen et al. \(1995, 1998\)](#) and will be discussed later in this paper.

Here we extend this investigation to the case in which the system is coupled to several thermal reservoirs at different temperatures. Remarkably, we find, for the first time we believe, a Lyapunov functional for such systems. This is described in Sections 2 and 3. Then in Section 4 we consider entropy production for such systems, and in Section 5 we consider the presence of an external electric field. Finally, in Section 6 we consider the possibility of deriving such kinetic models from more microscopic descriptions.

### 1.1 Description of the basic model

As already indicated, we deal in this note with a system described by the one-particle probability density  $f(v, t)$ . We are interested in particular in the case in which the evolution is given by the non-linear Boltzmann equation with pseudo-Maxwellian molecular collisions, for which the collision kernel is

$$Q(f, f) := \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} b\left(\frac{v - v_*}{|v - v_*|} \cdot \sigma\right) [f(v'_*)f(v') - f(v_*)f(v)] dv_* d\sigma.$$

Here  $d\sigma$  denotes the uniform probability measure on the sphere, and

$$v' := \frac{v + v_* + |v - v_*|\sigma}{2} \quad \text{and} \quad v'_* := \frac{v + v_* - |v - v_*|\sigma}{2}.$$

We assume *Grad’s angular cut-off* with  $\int_{\mathbb{S}^2} b(u \cdot \sigma) d\sigma = 1$  for any unit vector  $u$ , so that

$$\frac{1}{2} \int_{-1}^1 b(s) ds = 1. \tag{1.1}$$

Then we can separate  $Q(f, f)$  into its gain and loss terms

$$Q(f, f) = Q^+(f, f) - Q^-(f, f),$$

where

$$Q^+(f, g)(v) := \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} b\left(\frac{v - v_*}{|v - v_*|} \cdot \sigma\right) g(v'_*)f(v') dv_* d\sigma, \tag{1.2}$$

$$Q^-(f, g) := f.$$

Observe that the equilibria canceling this collision operator are given by the so-called Maxwellian density

$$M_{u,T}(v) := \frac{1}{(2T\pi)^{3/2}} \exp\left(-\frac{|v - u|^2}{2T}\right)$$

with bulk velocity  $u \in \mathbb{R}^3$ , and temperature  $T > 0$ . We denote simply  $M_T = M_{0,T}$  when  $u = 0$ .

The system is spatially homogeneous, and is coupled to several thermal reservoirs, indexed by  $\alpha$ , at temperatures  $T_\alpha$ . To describe the interaction with the reservoirs, we include in the evolution equation a term of the form  $Q(f, R)$ . The simplest example would have two reservoirs at temperatures  $T_1$  and  $T_2$  with the same coupling, in which case

$$R := \frac{1}{2}M_{T_1} + \frac{1}{2}M_{T_2}. \tag{1.3}$$

However, our methods and results do not depend very much on this particular form of  $R$ , and for this reason we leave the distribution  $R$  unspecified in much of our discussion.

It will be convenient to choose the time scale so that the total loss term coming from both  $Q(f, f)$  and  $Q(f, R)$  is simply  $-f$ . We can do this whatever the relative strength of the two collision mechanisms by making an appropriate choice of the time scale so that in terms of a parameter  $\gamma \in (0, 1)$ , the evolution equation can be written as

$$\frac{\partial f}{\partial t} = (1 - \gamma)Q(f, f) + \gamma Q(f, R), \tag{1.4}$$

where  $R$  be any given probability density on  $\mathbb{R}^3$ . Of course, if  $R = M_T$  for some  $T$ , then  $M_T$  is the unique steady state solution of (1.4). However, if  $R$  is given by (1.3) for  $T_1 \neq T_2$ , then we have no simple expression for any steady state.

Without loss of generality, we can scale the energy such that

$$\int_{\mathbb{R}^3} vR(v) dv = 0 \quad \text{and} \quad \int_{\mathbb{R}^3} |v|^2 R(v) dv = 1. \tag{1.5}$$

**Lemma 1.1.** *Let  $f_\infty$  be any steady-state probability density of (1.4). Then, assuming (1.5), we have*

$$\int_{\mathbb{R}^3} v f_\infty(v) dv = 0 \quad \text{and} \quad \int_{\mathbb{R}^3} |v|^2 f_\infty(v) dv = 1.$$

**Proof.** Let  $f$  be a solution of (1.4). For any test function  $\varphi(v)$ , and any two probability densities  $f$  and  $g$ , we have, by a standard computation

$$\int_{\mathbb{R}^3} Q(f, g)\varphi(v) dv = \int_{\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{S}^2} b(\sigma \cdot k) f(v)g(v_*)[\varphi(v') - \varphi(v)] dv dv_* d\sigma,$$

where  $k := |v - v_*|^{-1}(v - v_*)$ .

For  $\varphi(v) = v$ ,  $\varphi(v') - \varphi(v) = \frac{1}{2}(v_* - v + |v_* - v|\sigma)$ . Decomposing  $\sigma = (\sigma \cdot k)k + \sigma^\perp$ , we have that

$$\begin{aligned} & \int_{\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{S}^2} b(\sigma \cdot k) f(v) f(v_*)[\varphi(v') - \varphi(v)] dv dv_* d\sigma \\ &= \left[ 1 - \frac{1}{2} \int_{-1}^1 s b(s) ds \right] \int_{\mathbb{R}^3 \times \mathbb{R}^3} \left( \frac{v_* - v}{2} \right) f(v) g(v_*) dv dv_*. \end{aligned}$$

Therefore,

$$\begin{aligned} \frac{d}{dt} \left( \int_{\mathbb{R}^3} f(t, v) v \, dv \right) &= \gamma \int_{\mathbb{R}^3} Q(f, R) v \, dv \\ &= -\frac{\gamma}{2} \left[ 1 - \frac{1}{2} \int_{-1}^1 sb(s) \, ds \right] \int_{\mathbb{R}^3} f(t, v) v \, dv. \end{aligned}$$

By (1.1),  $[1 - \frac{1}{2} \int_{-1}^1 sb(s) \, ds] > 0$ , and so the first moment relaxes to zero exponentially fast.

Likewise, for  $\varphi(v) = |v|^2$ ,

$$\varphi(v') - \varphi(v) = \frac{|v_*|^2 - |v|^2}{2} - \sigma \cdot (v + v_*).$$

Decomposing  $\sigma$  as before,

$$\begin{aligned} &\int_{\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{S}^2} b(\sigma \cdot k) f(v) f(v_*) [\varphi(v') - \varphi(v)] \, dv \, dv_* \, d\sigma \\ &= \left[ 1 - \frac{1}{2} \int_{-1}^1 sb(s) \, ds \right] \int_{\mathbb{R}^3 \times \mathbb{R}^3} \left( \frac{|v_*|^2 - |v|^2}{2} \right) f(v) g(v_*) \, dv \, dv_*. \end{aligned}$$

Therefore,

$$\begin{aligned} \frac{d}{dt} \left( \int_{\mathbb{R}^3} f(t, v) |v|^2 \, dv \right) &= \gamma \int_{\mathbb{R}^3} Q(f, R) |v|^2 \, dv \\ &= -\frac{\gamma}{2} \left[ 1 - \frac{1}{2} \int_{-1}^1 sb(s) \, ds \right] \left( \int_{\mathbb{R}^3} f(t, v) |v|^2 \, dv - 1 \right). \end{aligned}$$

It follows that  $(\int_{\mathbb{R}^3} f(t, v) |v|^2 \, dv - 1)$  relaxes to zero exponentially fast. In any steady state, these moments must have the limiting value.  $\square$

### 1.2 The fixed-point equation

Because we have fixed the time scale so that the total loss term is simply  $f$ , the steady-state equation can be written as

$$f = (1 - \gamma) Q^+(f, f) + \gamma Q^+(f, R).$$

We now follow a method introduced in Carlen et al. (2000) to solve this equation.

Define the function  $\Phi$  from the space of probability densities on  $\mathbb{R}^3$  into itself by

$$\Phi(f) = (1 - \gamma) Q^+(f, f) + \gamma Q^+(f, R) \tag{1.6}$$

so that the steady-state equation is simply

$$f = \Phi(f). \tag{1.7}$$

We shall show that  $\Phi$  is contractive in the Gabetta–Toscani–Wennberg metric (Gabetta et al. (1985)), which is the metric defined as follows: Let  $f$  and  $g$  be two probability densities on  $\mathbb{R}^3$  with finite second moments such that the first and second moments are identical. Let  $\widehat{f}$  and  $\widehat{g}$  denote their Fourier transforms. Then

$$d_{\text{GTW}}(f, g) := \sup_{\xi \neq 0} \frac{|\widehat{f}(\xi) - \widehat{g}(\xi)|}{|\xi|^2}.$$

The following contraction lemma gives us existence and uniqueness of steady states for (1.4).

**Lemma 1.2.** *For all probability densities  $f$  and  $g$  with the same first and second moments as  $R$ ,*

$$d_{\text{GTW}}(\Phi(f), \Phi(g)) \leq \left(1 - \gamma \left[\frac{1}{2} - \frac{1}{4} \int_{-1}^1 sb(s) ds\right]\right) d_{\text{GTW}}(f, g).$$

In particular, if  $b$  is even,

$$d_{\text{GTW}}(\Phi(f), \Phi(g)) \leq \left(1 - \frac{\gamma}{2}\right) d_{\text{GTW}}(f, g).$$

**Proof.** Recall the Bobylev formula (Bobylev (1975, 1988)),

$$\widehat{Q}^+(f, g)(\xi) = \int_{\mathbb{S}^2} \widehat{f}(\xi_+) \widehat{g}(\xi_-) b\left(\sigma \cdot \frac{\xi}{|\xi|}\right) d\sigma, \tag{1.8}$$

where

$$\xi_{\pm} = \frac{\xi \pm |\xi|\sigma}{2}. \tag{1.9}$$

Note that  $|\xi_+|^2 + |\xi_-|^2 = |\xi|^2$ .

Then we decompose

$$\widehat{Q}^+(f, f) - \widehat{Q}^+(g, g) = \widehat{Q}^+(f - g, f) + \widehat{Q}^+(g, f - g)$$

and we deduce

$$\begin{aligned} d_{\text{GTW}}(Q^+(f, f), Q^+(g, g)) &= \sup_{\xi \neq 0} \frac{|\widehat{Q}^+(f - g, f) + \widehat{Q}^+(g, f - g)|}{|\xi|^2} \\ &\leq \sup_{\xi \neq 0} \int_{\mathbb{S}^2} \frac{|\widehat{f} - \widehat{g}|(\xi_+) |\widehat{g}|(\xi_-)}{|\xi|^2} b\left(\sigma \cdot \frac{\xi}{|\xi|}\right) d\sigma \\ &\quad + \sup_{\xi \neq 0} \int_{\mathbb{S}^2} \frac{|\widehat{g}|(\xi_+) |\widehat{f} - \widehat{g}|(\xi_-)}{|\xi|^2} b\left(\sigma \cdot \frac{\xi}{|\xi|}\right) d\sigma. \end{aligned}$$

Next, using the definition of  $d_{\text{GTW}}(f, g)$  and the fact that  $\|\widehat{g}\|_\infty \leq 1$ ,

$$\begin{aligned} & \int_{\mathbb{S}^2} \frac{|\widehat{f} - \widehat{g}|(\xi_+) |\widehat{g}|(\xi_-)}{|\xi|^2} b\left(\sigma \cdot \frac{\xi}{|\xi|}\right) d\sigma \\ &= \int_{\mathbb{S}^2} \frac{|\widehat{f} - \widehat{g}|(\xi_+) |\widehat{g}|(\xi_-) |\xi_+|^2}{|\xi_+|^2 |\xi|^2} b\left(\sigma \cdot \frac{\xi}{|\xi|}\right) d\sigma \\ &\leq d_{\text{GTW}}(f, g) \int_{\mathbb{S}^2} \frac{|\xi_+|^2}{|\xi|^2} b\left(\sigma \cdot \frac{\xi}{|\xi|}\right) d\sigma. \end{aligned}$$

Likewise,

$$\sup_{\xi \neq 0} \int_{\mathbb{S}^2} \frac{|\widehat{g}|(\xi_+) |\widehat{f} - \widehat{g}|(\xi_-)}{|\xi|^2} b\left(\sigma \cdot \frac{\xi}{|\xi|}\right) d\sigma \leq d_{\text{GTW}}(f, g) \int_{\mathbb{S}^2} \frac{|\xi_-|^2}{|\xi|^2} b\left(\sigma \cdot \frac{\xi}{|\xi|}\right) d\sigma.$$

Then since  $|\xi_+|^2 + |\xi_-|^2 = |\xi|^2$ , we have that

$$d_{\text{GTW}}(Q^+(f, f), Q^+(g, g)) \leq d_{\text{GTW}}(f, g).$$

Next, by essentially the same calculation,

$$\begin{aligned} d_{\text{GTW}}(Q^+(f, R), Q^+(g, R)) &\leq \int_{\mathbb{S}^2} \frac{|\widehat{f} - \widehat{g}|(\xi_+) |\widehat{R}|(\xi_-) |\xi_+|^2}{|\xi_+|^2 |\xi|^2} b\left(\sigma \cdot \frac{\xi}{|\xi|}\right) d\sigma \\ &\leq d_{\text{GTW}}(f, g) \int_{\mathbb{S}^2} \frac{|\xi_+|^2}{|\xi|^2} b\left(\sigma \cdot \frac{\xi}{|\xi|}\right) d\sigma. \end{aligned}$$

Since  $|\xi_+|^2 = \frac{1}{2}(|\xi|^2 + |\xi|(\xi \cdot \sigma))$ ,

$$\int_{\mathbb{S}^2} \frac{|\xi_+|^2}{|\xi|^2} b\left(\sigma \cdot \frac{\xi}{|\xi|}\right) d\sigma = \frac{1}{4} \int_{-1}^1 (1+s)b(s) ds.$$

Altogether, by the triangle inequality, we have

$$d_{\text{GTW}}(\Phi(f, f), \Phi(g, g)) \leq \left( (1-\gamma) + \gamma \left[ \frac{1}{4} \int_{-1}^1 (1+s)b(s) ds \right] \right) d_{\text{GTW}}(f, g),$$

which gives the result. □

**Theorem 1.3.** *Suppose that  $R$  satisfies (1.5). Then there is a unique steady-state solution  $f_\infty$  of (1.4). Moreover, if we define a sequence by  $f_0 = R$  and  $f_n = \Phi(f_{n-1})$  for all  $n \in \mathbb{N}$ , then  $f_\infty = \lim_{n \rightarrow \infty} f_n$ , and*

$$d_{\text{GTW}}(f_n, f_\infty) \leq \frac{\lambda^n}{1-\lambda} d_{\text{GTW}}(\Phi(R), R), \tag{1.10}$$

where

$$\lambda = \left( (1-\gamma) + \gamma \left[ \frac{1}{4} \int_{-1}^1 (1+s)b(s) ds \right] \right) < 1.$$

**Proof.** This is a direct consequence of the previous lemma and the contraction mapping theorem. Recall from the proof that

$$d_{\text{GTW}}(f_{n+1}, f_n) \leq \lambda^n d_{\text{GTW}}(\Phi(R), R).$$

Then by the triangle inequality we obtain the final estimate. □

We remark that the equation (1.10) allows the effective computation of  $f_\infty$ . Once can certainly evaluate it numerically, especially when  $b$  is even so that  $\lambda = 1 - \gamma/2$ .

## 2 Exponential convergence

Since for small  $h$ , and any two solutions  $f$  and  $g$  of (1.4),

$$f(t+h) - g(t+h) = h[\Phi(f(t)) - \Phi(g(t))] + (1-h)[f(t) - g(t)] + o(h),$$

it follows from our contraction estimate in the previous section that provided  $f(0)$  and  $g(0)$  have the same first and second moments as  $R$ ,

$$\begin{aligned} & \frac{d}{dt} d_{\text{GTW}}(f(t), g(t)) \\ & \leq - \left[ 1 - \left( (1-\gamma) + \gamma \left[ \frac{1}{4} \int_{-1}^1 (1+s)b(s) ds \right] \right) \right] d_{\text{GTW}}(f(t), g(t)). \end{aligned}$$

In particular, taking  $g(t) = f_\infty$ , we see that  $d_{\text{GTW}}(f(t), f_\infty)$  decreases to zero exponentially fast.

We can dispense with the requirement that the initial data  $f(0)$  has the same first and second moments as  $R$  by using the correction technique introduced in Carlen et al. (1999). Let us describe briefly this argument. Let us denote

$$\begin{aligned} \lambda_0 & := \frac{1}{2} \left[ 1 - \frac{1}{2} \int_{-1}^{+1} sb(s) ds \right] > 0, \\ \lambda_1 & := \left[ 1 - \left( (1-\gamma) + \gamma \left[ \frac{1}{4} \int_{-1}^1 (1+s)b(s) ds \right] \right) \right] > 0. \end{aligned}$$

We define (in Fourier variables)

$$\widehat{\mathcal{M}}[f] := \chi(\xi) \sum_{|\alpha| \leq 2} \left( \int_{\mathbb{R}^3} v^\alpha f(v) dv \right) \frac{\xi^\alpha}{\alpha!},$$

where we use the standard notation for multi-indices  $\alpha = (\alpha_1, \alpha_2, \alpha_3) \in \mathbb{N}^3$ ,  $|\alpha| = \alpha_1 + \alpha_2 + \alpha_3$ ,  $v^\alpha = v_1^{\alpha_1} v_2^{\alpha_2} v_3^{\alpha_3}$ ,  $\alpha! = \alpha_1! \alpha_2! \alpha_3!$ , and where  $\chi$  is a compactly supported smooth function that is equal to one around  $\xi = 0$ . Then if we consider two solutions  $f$  and  $g$  with possibly different momentum and energy, we write  $D = f - g - \mathcal{M}[f - g]$ ,  $S = f + g$ , and obtain

$$\partial_t D = (1 - \gamma)Q(D, S) + (1 - \gamma)Q(S, D) + \gamma Q(D, R) - W$$

with

$$W := [\partial_t \mathcal{M}[f - g] + (1 - \gamma) \mathcal{Q}(\mathcal{M}[f - g], S) + (1 - \gamma) \mathcal{Q}(S, \mathcal{M}[f - g]) + \gamma \mathcal{Q}(\mathcal{M}[f - g], R)],$$

and one checks by similar moment estimates as above that

$$|\widehat{W}(\xi, t)| \leq C |\xi|^2 \left( \sum_{|\alpha| \leq 2} \left| \int_{\mathbb{R}^3} v^\alpha [f(v, t) - g(v, t)] dv \right| \right) \leq C' |\xi|^2 e^{-\lambda_0 t}$$

for some constants  $C, C' > 0$ . We then perform the same contraction estimate as before since  $D$  is now the Fourier transform of a centered zero-energy function, and obtain

$$\sup_{\xi \in \mathbb{R}^3} \frac{|\widehat{D}(\xi, t)|}{|\xi|^2} \leq \sup_{\xi \in \mathbb{R}^3} \frac{|\widehat{D}(\xi, 0)|}{|\xi|^2} e^{-\lambda_1 t} + C'' e^{-\min(\lambda_0, \lambda_1) t}$$

for some constant  $C_1$ . Finally, we deduce by taking  $g = f_\infty$  that  $f$  is converging to the equilibrium  $f_\infty$  with exponential rate, measured in the distance

$$d'_{\text{GTW}}(f, g) = \sup_{\xi \in \mathbb{R}^3} \frac{|\widehat{f}(\xi) - \widehat{g}(\xi) - \widehat{\mathcal{M}}[f - g](\xi)|}{|\xi|^2} + |\mathcal{M}[f - g]|,$$

which writes  $d'_{\text{GTW}}(f, f_\infty) \leq C''' e^{-\min(\lambda_0, \lambda_1) t}$  for some constant  $C''' > 0$ .

### 3 Diffusive thermal reservoirs

In some physical situations, it is more appropriate to model the interaction of a system with reservoirs by an Ornstein–Uhlenbeck continuous time process rather than the discrete time collision model that we have considered above. This leads to a kinetic equation of the form

$$\frac{\partial}{\partial t} f(v, t) = Q(f, f) + \sum_{\alpha} \eta_{\alpha} T_{\alpha} \frac{\partial}{\partial v} \left[ M_{T_{\alpha}} \frac{\partial}{\partial v} \left( \frac{f}{M_{T_{\alpha}}} \right) \right]. \tag{3.1}$$

The constant  $\eta_{\alpha}$  sets the strength of the interaction with the  $\alpha$ th reservoir.

Note that in this setting, the evolution equation for several reservoirs reduces to the evolution equation for a single reservoir, since

$$\sum_{\alpha} \eta_{\alpha} T_{\alpha} \frac{\partial}{\partial v} \left[ M_{T_{\alpha}} \frac{\partial}{\partial v} \left( \frac{f}{M_{T_{\alpha}}} \right) \right] = \eta T \frac{\partial}{\partial v} \left[ M_T \frac{\partial}{\partial v} \left( \frac{f}{M_T} \right) \right],$$

where

$$\eta = \sum_{\alpha} \eta_{\alpha} \quad \text{and} \quad T = \frac{1}{\eta} \sum_{\alpha} \eta_{\alpha} T_{\alpha}.$$



The effective evolution equation

$$\frac{\partial f}{\partial t} = Q(f, f) + \eta T \frac{\partial}{\partial v} \left[ M_T \frac{\partial}{\partial v} \left( \frac{f}{M_T} \right) \right] \tag{3.2}$$

is then easy to analyze since in this case the unique stationary state is  $M_T$ , and the relative entropy with respect to  $M_T$ , that is,  $\int_{\mathbb{R}^3} f [\log f - \log M_T] dv$  decreases to zero exponentially fast. Likewise,

$$\left[ 3T - \int_{\mathbb{R}^3} v^2 f(v, t) dv \right] = e^{-2\eta t} \left[ 3T - \int_{\mathbb{R}^3} v^2 f(v, 0) dv \right].$$

In fact, more is true: This evolution also has the contractive property proved in the previous section for (1.4), now using a different metric, but one that is equivalent to the GTW metric (Gabetta et al. (1985)), namely the 2-Wasserstein metric.

A theorem of Tanaka (Tanaka (1973, 1978/1979)) says that the evolution described by the spatially homogeneous Boltzmann equation for Maxwellian molecules is contractive in this metric. (We do not describe this metric here, other than to say that like the GTW metric, it metrizes the topology of weak convergence of probability measures together with convergence of second moments, and we refer to the book Villani (2003) for the definition and the proof of this fact.)

As Otto has shown (Otto (2001)), the evolution described by

$$\frac{\partial f}{\partial t} = \eta T \frac{\partial}{\partial v} \left[ M_T \frac{\partial}{\partial v} \left( \frac{f}{M_T} \right) \right]$$

is exponentially contractive in the 2-Wasserstein metric: If  $f$  and  $g$  are any two solutions of this equation

$$d_{W_2}(f(\cdot, t), g(\cdot, t)) \leq e^{-\eta(t-s)} d_{W_2}(f(\cdot, s), g(\cdot, s)).$$

Together with Tanaka’s theorem for the equation with the collision operator  $Q$  only and a splitting argument (i.e., a non-linear Trotter product argument), one easily establishes that this same estimate is valid for solutions of (3.2) and therefore (3.1). In particular, it follows that for all solutions  $f(v, t)$  of (3.1),

$$\begin{aligned} d_{W_2}(f(\cdot, t), M_T) &\leq e^{-\eta t} d_{W_2}(f(\cdot, 0), M_T) \\ &\leq e^{-(\eta/T)t} \left( \frac{1}{2} \int v^2 f(v, 0) dv + T \right), \end{aligned} \tag{3.3}$$

where we have used a simple estimate (see Villani (2003)) for  $d_{W_2}(f(\cdot, 0), M_T)$  in the last inequality.

In conclusion, for the diffusive reservoirs, we have not only a “free energy type” Lyapunov functional, namely the relative entropy with respect to  $M_T$ , but also a different one that is similar in nature to the one we found in the previous section for (1.4).

#### 4 Entropy production for thermal reservoirs

We now consider the entropy production when the reservoirs are thermal. More precisely, we assume that the time evolution of  $f(v, t)$  is given by

$$\frac{\partial f}{\partial t} = Q(f, f) + \sum_{\alpha} \int_{\mathbb{R}^3} [K_{\alpha}(v, v')f(v') - K_{\alpha}(v', v)f(v)] dv'. \quad (4.1)$$

The Markovian rates  $K_{\alpha}(v, v')$  describe collisions with the thermal reservoir at temperature  $T_{\alpha} = \beta_{\alpha}^{-1}$  resulting in a transition from  $v'$  to  $v$ , and  $Q(f, f)$  is a general Boltzmann type collision operator, not necessarily of the Maxwellian type. We assume detailed balance for each reservoir; that is,

$$\forall \alpha, \quad K(v, v')M_{T_{\alpha}}(v') = K(v', v)M_{T_{\alpha}}(v). \quad (4.2)$$

Equations (4.1) and (4.2) thus include (1.4) and (1.3) as special cases. However, the exponential approach proved for the latter may not hold in this more general case. In fact, even the existence and uniqueness of a stationary state for (4.1) and (4.2) is not guaranteed; see, for example, Carlen et al. (1995, 1998). On the other hand, the analysis below applies to the broader class of models for which there is existence and uniqueness of the NESS, and also carries over to the case in which  $f$  and the  $K_{\alpha}$  depend on position  $x \in \mathbb{R}^3$ , though we shall not pursue this here.

The rate of change of the system's Boltzmann gas entropy is given by

$$\dot{S} = -\frac{d}{dt} \int_{\mathbb{R}^3} f \log f dv = \sigma_B + \sum_{\alpha} \sigma_{\alpha} - \sigma_R, \quad (4.3)$$

where  $\sigma_B$  is the usual rate of change of the entropy due to the Boltzmann collision term, which is non-negative and equal to zero if and only if  $f$  is a Maxwellian. The  $\sigma_{\alpha}$  are given by

$$\begin{aligned} \sigma_{\alpha} &:= \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} K_{\alpha}(v, v') M_{\alpha}(v') [v_{\alpha}(v, t) - v_{\alpha}(v', t)] \log \frac{v_{\alpha}(v, t)}{v_{\alpha}(v', t)} dv dv' \\ &\geq 0, \end{aligned} \quad (4.4)$$

where

$$v_{\alpha}(v, t) = \frac{f(v, t)}{M_{\alpha}(v)}.$$

Finally,  $\sigma_R$  is the rate of production of entropy in the reservoirs

$$\sigma_R := \sum_{\alpha} \beta_{\alpha} J_{\alpha} \quad (4.5)$$

with

$$J_{\alpha}(t) := \frac{1}{2} \int \int K_{\alpha}(v, v') f(v', t) [v'^2 - v^2] dv dv' \quad (4.6)$$

being the flux of energy into the  $\alpha$ th reservoir at time  $t$ .

The total rate of entropy production in the system plus reservoirs is given by

$$\sigma = \dot{S} + \sum_{\alpha} \beta_{\alpha} J_{\alpha} \geq 0. \quad (4.7)$$

In the stationary state,  $\dot{S} = 0$ , and

$$\bar{\sigma} = \sum_{\alpha} \beta_{\alpha} \bar{J}_{\alpha} = \bar{\sigma}_B + \sum_{\alpha} \bar{\sigma}_{\alpha} \geq 0, \quad (4.8)$$

where the bars denote quantities computed in the stationary state  $f_{\infty}$ .

There is equality in (4.8) if and only if  $\bar{\sigma}_B = 0$  and  $\bar{\sigma}_{\alpha} = 0$  for each  $\alpha$ , and this is the case if and only if the stationary state is a Maxwellian, and all of the reservoirs have the same temperature.

In the case of equal temperature  $\beta_{\alpha} = \beta$  for all  $\alpha$ ,  $\sigma$  in (4.7) is given by

$$\sigma = \frac{d}{dt}[S - \beta\mathcal{E}] = -\beta \frac{d}{dt}\mathcal{F},$$

where  $\mathcal{E} = \frac{1}{2}\langle v^2 \rangle$  is the average energy of the system and  $\mathcal{F}$  is a kind of free energy.  $\mathcal{F}$  is thus a Lyapunov functional achieving its minimum when  $f = M_T$ . In fact, it is just the relative entropy of  $f$  with respect to  $M_T$ .

When the  $\beta_{\alpha}$  are unequal,  $\sigma$  is not a time derivative, and the only Lyapunov functionals we know are  $d_{\text{GTW}}(f, f_{\infty})$  (or  $d_{W_2}(f, f_{\infty})$  in the case of diffusive reservoirs), and only in the case in which the time evolution is given by (1.4).

In the stationary state, we must of course have  $\sum_{\alpha} \bar{J}_{\alpha} = 0$ . Hence if we have only two reservoirs, then

$$\bar{\sigma} = (\beta_1 - \beta_2)\bar{J}_1 \geq 0; \quad (4.9)$$

that is, heat flows from the hot to the cold reservoir.

We note that when the system is coupled to reservoirs (with equal or unequal temperatures), then  $S$  need not be monotone non-decreasing as is evident from the fact that we can start from an initial state with an entropy that is higher than that of the stationary state; for example, a Maxwellian with a sufficiently high temperature. It is only when  $\sigma_R \leq 0$  that  $\dot{S}$  must be non-negative.

The above considerations remain valid when the Boltzmann collision kernel  $Q(f, f)$  is replaced by the modified Enskog collision kernel which is generally considered to be a good approximation for a moderately dense gas; see Goldstein and Lebowitz (2003) and references provided there.

As noted above, in some physical situations it is more appropriate to model the interaction of a system with reservoirs by an Ornstein–Uhlenbeck continuous time diffusion process rather than a discrete time jump process as in (4.1). Our analysis of entropy production allows for a more general class of diffusive reservoirs than did our discussion of the contraction property. In particular, we can allow velocity dependent diffusion coefficients. Similarly, the collision term may be modified

when the system is not a dilute gas. We shall therefore write a general kinetic equation in the form

$$\frac{\partial f}{\partial t} = Q(f) + \sum_{\alpha} \frac{\partial}{\partial v} \left[ \eta_{\alpha}(v) T_{\alpha} M_{T_{\alpha}} \frac{\partial}{\partial v} \left( \frac{f}{M_{T_{\alpha}}} \right) \right] \tag{4.10}$$

requiring only that  $Q(f)$  conserve the energy, momentum and mass of  $f$ , and that

$$- \int_{\mathbb{R}^3} Q(f) \log f \, dv \geq 0$$

with equality if and only if  $f = M_T$  for some  $T$ . The above analysis can now be repeated with  $\sigma_{\alpha}$  replaced by

$$\sigma'_{\alpha} := \int_{\mathbb{R}^3} f \eta_{\alpha}(v) T_{\alpha} \left| \frac{\partial}{\partial v} \left( \frac{f}{M_{T_{\alpha}}} \right) \right|^2 \, dv.$$

### 5 Systems driven by an electric field

In the systems considered so far in this paper, a non-equilibrium steady state has been maintained by at least two reservoirs with energy flowing out of some and into others. A different sort of model is investigated in [Carlen et al. \(1995, 1998\)](#) which concerns a weakly ionized plasma with energy supplied by an electric field  $E$ , and removed into a reservoir by a damping mechanism. In this model, the probability density  $f(v, t)$  evolves according to

$$\frac{\partial f}{\partial t} = \frac{1}{\epsilon} Q(f) - E \cdot \frac{\partial}{\partial v} f + \nu [\tilde{f} - f] + \frac{\partial}{\partial v} \left[ D(v) M \frac{\partial}{\partial v} \left( \frac{f}{M} \right) \right]. \tag{5.1}$$

In (5.1),  $E$  is a constant electric field,  $\epsilon$  is a small parameter setting the rate of internal collisions,  $\tilde{f}$  is the spherical average of  $f$  (hence radial, but with the same energy distribution as  $f$ ),  $\nu$  is a constant, and  $M$  is a centered Maxwellian with  $T = 1$ . See (2.1-4) in [Carlen et al. \(1995\)](#).

When  $E = 0$ , the unique equilibrium is  $M$ , and the free energy  $\mathcal{F}$  is a Lyapunov function. Also when  $D(v) = D$  independent of  $v$ , and  $\nu = 0$ , the NESS is given by the shifted Maxwellian  $M(v - u)$  where  $u = ET/D$ . In this case

$$\mathcal{F} = \frac{1}{2} \langle |v - u|^2 \rangle - \beta S$$

serves as a Lyapunov function governing convergence to the NESS.

However, when  $D(v)$  has certain properties,  $E \neq 0$  and  $\nu > 0$ , it is shown in [Carlen et al. \(1995, 1998\)](#) that for all  $\epsilon$  sufficiently small, there is a range of the parameters for which there are multiple stable stationary solutions of (5.1). This means in particular that there does not exist any global Lyapunov function for (5.1) for general parameters.

Finally, we have in this stationary state that

$$\bar{\sigma} = \beta \bar{j} \cdot E \quad \text{where } \bar{j} = \int_{\mathbb{R}^3} v f_{\infty}(v) \, dv$$

is the steady-state current.

## 6 Microscopic models

We have investigated here the approach to the NESS and some properties of that state for models in contact with several thermal reservoirs at different temperatures. We showed that there exist in some cases Lyapunov functionals even when we do not know the NESS in explicit form. It would be nice to show that these models correspond to  $N$ -particle microscopic models in some suitable scaling limits.

A plausible conjecture is the following: Suppose that the dynamics of the isolated system is given by a Hamiltonian microscopic dynamics, and it yields, in some suitable limit, a Boltzmann equation for the single particle distribution; for example, hard-sphere collisions under the Boltzmann–Grad scaling limit (Lanford (1976), Gallagher et al. (2014), Pulvirenti et al. (2014)). Adding stochastic interactions with thermal reservoirs should then lead, in a suitable limit, to (4.1).

However, this is beyond our current reach, even for the case in which the system is in contact with a single reservoir. If one drops the requirement that the microscopic dynamics be Hamiltonian, the situation is much better. Such a microscopic derivation was proven recently by Bonetto, Loss and Vaidyanathan (2014) when the isolated system dynamics is given by the Kac stochastic collision model and there is a single thermal reservoir. One may expect a similar result to be valid for the Kac system in contact with several reservoirs.

## Acknowledgments

This paper may be reproduced, in its entirety, for non-commercial purposes. Work of E. A. Carlen is partially supported by NSF Grant DMS 1201354. J. L. Lebowitz wishes to thank the IAS its hospitality during the course of the work, and his work is partially supported by NSF Grant DMR 1104500 and AFOSR Grant FA9550. C. Mouhot wishes to thank the IAS for its support during his visit in may 2014 when this work was done. His research is also partially funded by the ERC Starting Grant MATKIT.

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