Nonequilibrium stationary states for some Model Systems

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Outline: There are different ways of modeling systems in nonequilibrium stationary states (NESS). I shall consider three.

(I) System interacts with its surroundings via a potential.

$$H_{\text{tot.}} = H_s + \sum_\alpha V_{S,R} + \sum_\alpha H_{R_\alpha}, \quad \alpha = 1, \dots, k$$

Time evolution can be classical or quantum.

(II) System is acted on by its surroundings via stochastic terms, e.g. Langevin forces.

(III) System evolves according to deterministic non-Hamiltonian dynamics, e.g. Gaussian thermostat.

Let me begin by describing some results in a paper that Herbert Spohn and I wrote together almost 40 years ago about a very idealized situation: *Comm. Math. Phys. (1977)*. I think that it is still of some interest today. Extensions to more realistic systems is still "work in progress".

In that paper we study the NESS of an infinite harmonic system. For simplicity we considered mostly a classical harmonic chain, which can be divided implicitly or explicitly into three parts:

semi-infinite left and right parts which act as infinite thermal reservoirs at temperatures T_L and T_R and a finite middle piece considered as our system S.

T_L λ S λ T_R

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We can equally well consider a system with finite cross section in directions perpendicular to the x-axis. The results are essentially the same.

The time evolution of the infinite system is Hamiltonian (or Schrödinger). The temperature of the left and right infinite parts is specified by choosing an initial non-equilibrium state μ_i in which the "left" and "right" parts of the infinite crystal are in "equilibrium" at different temperatures, $T_L = \beta_L^{-1} \neq \beta_R^{-1} = T_R$, and the "middle" part is in an arbitrary state. Starting with the initial distribution μ_i we proved that in the limit $t \to \infty$, μ approaches a unique stationary state which is independent of the initial system state. This state is Gaussian with a covariance matrix which satisfies a simple equation. One solution of that equation is the usual Gibbs measure with parameter β. It is the one approached when $\beta_L = \beta_R = \beta$.

For $\beta_L \neq \beta_R$ this state will not be Gibbsian. It will however be a translation invariant nonequilibrium stationary state (NESS) in which the mean kinetic energy of a particle of any fixed position will be $(T_L + T_R)/2$. Assuming $T_L > T_R$ this NESS will carry a heat current J from left to right which is proportional to $(T_L - T_R)$.

Since the system is translation invariant there will be no temperature gradient and thus no Fourier's Law. We do however have that $\sigma = \frac{J}{T_R} - \frac{J}{T_L} > 0$, when $T_L > T_R$. This σ can be interpreted as the "entropy production" in the "reservoirs". The system being a superconductor there will be no entropy production in the bulk.

Similar states are obtained for other (integrable) systems, such as free Fermions (or even interacting ones) started in pure states or density matrices with different chemical potentials on the left and the right where the “flat” steady state carries a particle current.

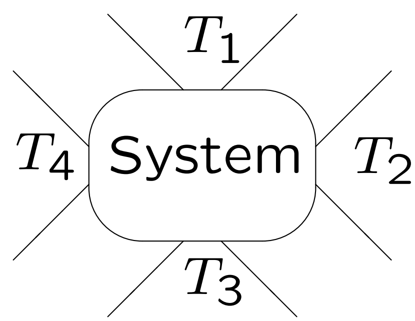
Quoting from the abstract of the paper: "We also investigate the limit of these stationary ($t \to \infty$) states as the coupling strength λ between the "system" and the "reservoirs" goes to zero. In this limit we obtain a product state, where the reservoirs are in equilibrium at temperatures β_L^{-1} and β_R^{-1} and the system is in the unique stationary state of the reduced dynamics in the weak coupling limit."

I will come back later to the weak coupling or Van Hove limit, in which one looks at long time scales $\tau = t/\lambda^2$ where t is the microscopic time scale and λ is the strength of the coupling between the system and its surroundings.

For the moment let me consider a simplified version of such models in which the interaction with the reservoirs is replaced by stochastic thermostat at specified temperatures.

Systems in Contact with Thermal Reservoirs

Consider a classical system with Hamiltonian $H(X)$, in contact with k thermal reservoirs at its boundaries. It is convenient to represent the reservoirs by stochastic (boundary) terms. This is clearly an idealization: it implies in particular that there is no influence from the system on the state of the reservoirs as far as their <u>future</u> effect on the system goes. This is certainly reasonable for modeling infinite, non-interacting particle / phonon / photon reservoirs.



For more realistic reservoirs, the situation is much more complicated and is an active area of research, especially for quantum systems (Froehlich, Kupiainen).

Let the αth reservoir, at temperature $T_\alpha = \beta_\alpha^{-1}$, act on the system impulsively by producing "jumps" from X' to X at a rate $K_\alpha(X, X')$. The ensemble (probability) density $\mu_t(X)$ will satisfy the Markovian evolution equation (master equation)

$$\frac{\partial \mu_t(X)}{\partial t} = (H, \mu_t) + \sum_\alpha \int \left[K_\alpha(X, X')\mu_t(X') - K_\alpha(X', X)\mu_t(X) \right] dX'. \quad (1)$$

We assume that if there was only one reservoir at temperature T_α, then the stationary state of the system would be given by the canonical distribution

$$\overline{\mu}_\alpha \sim e^{-\beta_\alpha H(X)}. \quad (2)$$

Note: H needs to be modified for realistic situations to include the effect of the system-reservoir interactions.

Detailed balance for transitions caused by the αth reservoir then corresponds to

$$e^{-\beta_\alpha H(X')} K_\alpha(X, X') = e^{-\beta_\alpha H(X)} K_\alpha(X', X), \tag{3}$$

This, together with general ergodicity conditions on K_α, will ensure that $\bar{\mu}_\alpha$ is indeed the only stationary state for a single reservoir. More generally, the requirement of ergodicity and that

$$\int \left[K_\alpha(X, X') e^{-\beta_\alpha H(X')} - K_\alpha(X', X) e^{-\beta_\alpha H(X)} \right] dX' = 0 \tag{4}$$

is sufficient for having the canonical (grand-canonical) ensemble density be the unique stationary state of the system when it is in contact with only the αth reservoir. A simple example where (4) holds but (3) does not is to add to the K_α satisfying an exchange of velocities, e.g. with a rate r

$\mathbf{v}_i \to \mathbf{v}_{j(i)} \to \mathbf{v}_{k(j)} \to \mathbf{v}_i$ according to some rule.

Entropy Production

The Gibbs entropy of the system at time t is given by

$$S_G(\mu_t) = -\int \mu_t \log \mu_t dX. \tag{5}$$

This quantity is no longer conserved by the evolution as it is for an isolated system, but its change does not have a definite sign. What is true however (and easy to show) is that

$$\sigma = \frac{dS_G}{dt} + \sum_{\alpha=1}^{k} \beta_\alpha J_\alpha \geq 0 \tag{6}$$

Here J_α is the flux of energy to the αth reservoir from the system

$$J_\alpha = \int dX \mu_t(X) \int \Big[H(X) - H(X')\Big] K_\alpha(X', X) dX', \tag{7}$$

and $\beta_\alpha J_\alpha$ may be interpreted as the rate of entropy production in the αth reservoir so that σ is the "total entropy production" in system plus reservoirs.

$$\sigma = \sum_{\alpha=1}^{k} \iint K_\alpha(X, X') e^{-\beta_\alpha H(X')} \times \left\{ \nu_\alpha(X') \left[\log \nu_\alpha(X') - \log \nu_\alpha(X) \right] - \nu_\alpha(X') + \nu_\alpha(X) \right\} dX dX' \geq 0 \tag{8}$$

where

$$\nu_\alpha(X) = e^{\beta_\alpha H(X)} \mu(X). \tag{9}$$

A similar result holds when the effect of the reservoirs is represented by Ornstein-Uhlenbeck processes:

$$\frac{d\mathbf{v}_i}{dt} = -\frac{\partial H}{\partial \mathbf{r}_i} + \sum_{\alpha=1}^{k} \left[-\lambda_i^\alpha \mathbf{v}_i \; + \sqrt{2\beta_\alpha^{-1}\lambda_i^\alpha}\mathcal{F}_i^\alpha(t) \right] \tag{10}$$

with

$$\left\langle \mathcal{F}_i^\alpha(t)\mathcal{F}_j^\gamma(t') \right\rangle = \delta_{i,j}\delta_{\alpha,\gamma}\delta(t-t'). \tag{11}$$

The master (Fokker-Planck) equation then takes the form

$$\frac{\partial \mu_t(X)}{\partial t} + (\mu_t, H) = \sum_{\alpha=1}^{k} \beta_\alpha^{-1} \sum_{i=1}^{N} \lambda_i^\alpha \frac{\partial}{\partial \mathbf{v}_i} \left[\overline{\mu}_\alpha \frac{\partial}{\partial \mathbf{v}_i} \left(\frac{\mu_t}{\overline{\mu}_\alpha} \right) \right]. \tag{12}$$

We then have

$$\sigma = \sum_\alpha \beta_\alpha^{-1} \sum_i \int \lambda_i^\alpha \left[\frac{\partial}{\partial \mathbf{v}_i} \log \nu_\alpha(X) \right]^2 \mu dX \geq 0. \tag{13}$$

We note that for the case of a single reservoir at temperature β_α^{-1}, σ is just the rate of change of the (negative) relative entropy w.r.t. the stationary state $\overline{\mu}$, $S_G(\mu|\overline{\mu}) = -\int \mu \log \frac{\mu}{\overline{\mu}}\, dX$. In the single reservoir case, $\overline{\mu} = \mu_\alpha \sim \exp[-\beta_\alpha H]$, and

$$\sigma = \frac{d}{dt} S_G(\mu_t|\mu_\alpha) = -\frac{d}{dt} F_G(t) \geq 0 \tag{14}$$

where

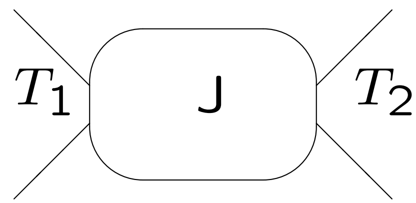
$$F_G(t) = \beta_\alpha \langle U \rangle_{\mu_t} - S_G(t). \tag{15}$$

This monotone increase in relative entropy is true for all Markov processes, but it does not in general help very much when the stationary state $\overline{\mu}$ is unknown.

In the stationary state

$$\frac{dS}{dt} = 0, \quad \frac{d\langle H\rangle}{dt} = -\sum J_\alpha = 0, \text{ and } \sigma_{\mathsf{st}} = \sum_{\alpha=1}^{k} \beta_\alpha J_\alpha \geq 0. \tag{16}$$

For $k = 1$, there is no net energy flow or entropy production in the stationary state, and so $\sigma_{\mathsf{st}} = 0$. This is true even in the absence of detailed balance for K_α.



For $k = 2$,

$$J_1 = -J_2 = -J \ \text{ and so } \ \sigma_{\text{st}} = J\left(\frac{1}{T_2} - \frac{1}{T_1}\right) \geq 0. \qquad (17)$$

It follows from this that the energy flow, if any, will be from the hotter to the cooler reservoir (from left to right for $T_1 > T_2$). For $k > 2$, there can be complex flow patterns of the energy in the stationary state (Eckman, et. al.).

But, how will the flux depend on the system Hamiltonian H and on the K_α's? In particular: will Fourier's Law hold? This is still very much an open question.

Thermostatted Systems

Gaussian Thermostats

An alternative to obtaining non-equilibrium stationary states (NESS) of a finite system by coupling it to infinite reservoirs is to consider (finite) systems with a deterministic evolution which is non-Hamiltonian.

A much studied example of such non-Hamiltonian dynamics is one with a Gaussian thermostat which keeps the kinetic energy of the system constant. While this dynamics is not very physical, it is mathematically interesting and can be related in many cases to physical behavior. In particular, it has led to rigorous theorems, such as the Gallavotti - Cohen fluctuation theorem for Anosov flows which appear to apply also to physical systems with Hamiltonian dynamics. It has also led to a proof of "Fourier's Law" for a chain of weakly coupled chaotic systems in which fluctuations in the kinetic energy of the chaotic elements is suppressed by the use of thermostats.

I will now describe some old and new results on the NESS of a multiparticle system moving among fixed scatterers subject to an external field, $\mathbf{E}$, and a Gaussian thermostat.

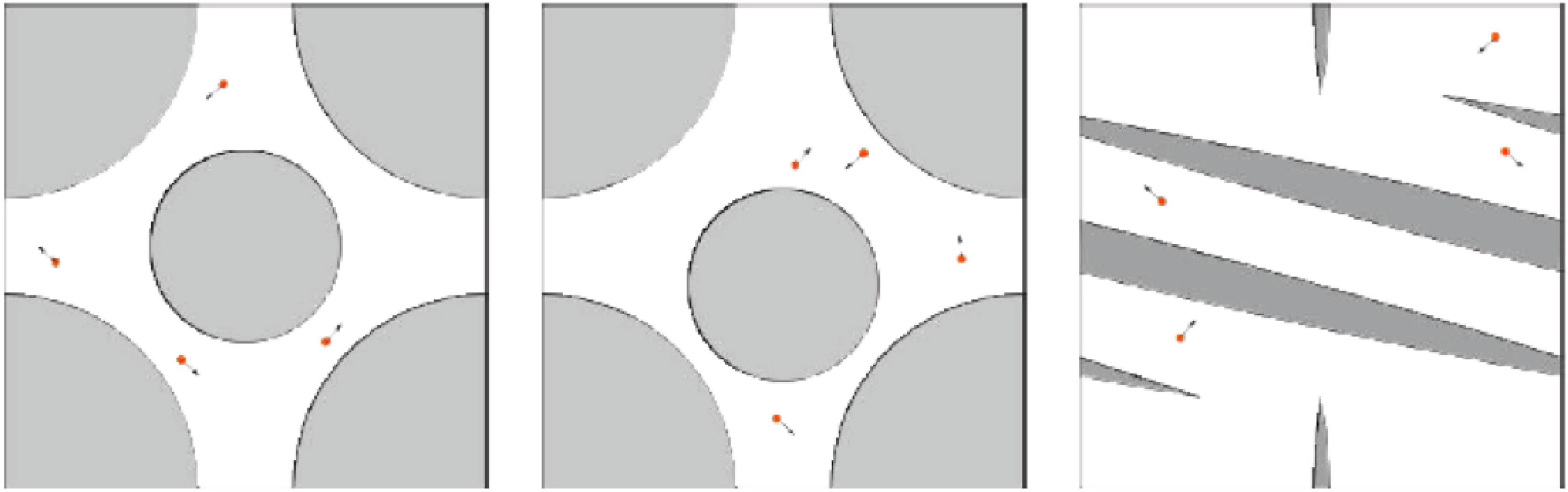


Table A Table B Table C

Different Sinai billiard tables.

The equations of motion of our system, consisting of N particles of mass 1 in a unit 2D torus, are

$$\begin{cases} \dot{\mathbf{q}}_i = \mathbf{v}_i \\ \dot{\mathbf{v}}_i = \mathbf{E} - \alpha(\mathbf{V}, K)\mathbf{v}_i + \mathbf{F}_i \end{cases} \qquad i = 1, 2, \ldots N \tag{18}$$

where $\mathbf{E}$ is the external field,

$$\alpha(\mathbf{V}, K) = \frac{(\mathbf{E} \cdot \mathbf{J})}{K}, \qquad \mathbf{J} = \sum_i \mathbf{v}_i, \qquad K = \sum_i |\mathbf{v}_i|^2 \tag{19}$$

and $\mathbf{F}_i$ is an impulsive change in the momentum of the i-th particle caused by its collision with a fixed scatterer, as in the figure. The term $\alpha(\mathbf{V}, K)$ represents the Gaussian thermostat which keeps K fixed. We may therefore set $K = N$. I shall refer to this system as the mechanical one (designated by M).

The Gaussian thermostat thus induces a "long range," "mean field" type of interaction between the particles: the speed gained by any particle due to the electric field has to be compensated by loss of speed in *all* the other particles due to the thermostatted "friction" α.

The one particle system, $N = 1$, first introduced by Moran and Hoover, has been investigated extensively both analytically and numerically. In particular, one can prove (Chernov, Eyink, L., Sinai), for small values of $\mathbf{E}$ (and magnetic field $\mathbf{B}$), that the system has a unique stationary SRB measure which is approached as $t \to \infty$ from any initial measure which is absolutely continuous w.r.t. Lebesgue measure.

This SRB measure, $\mu_{\mathbf{E}}^{+}$, is, however, singular w.r.t. Lebesgue measure. Its Hausdorff dimension is given for small $E = |\mathbf{E}|$ by

$$HD\left(\mu_{\mathbf{E}}^{+}\right) = 3 - \frac{\bar{\mathbf{J}} \cdot \mathbf{E}}{h_0} + o(E^2), \tag{20}$$

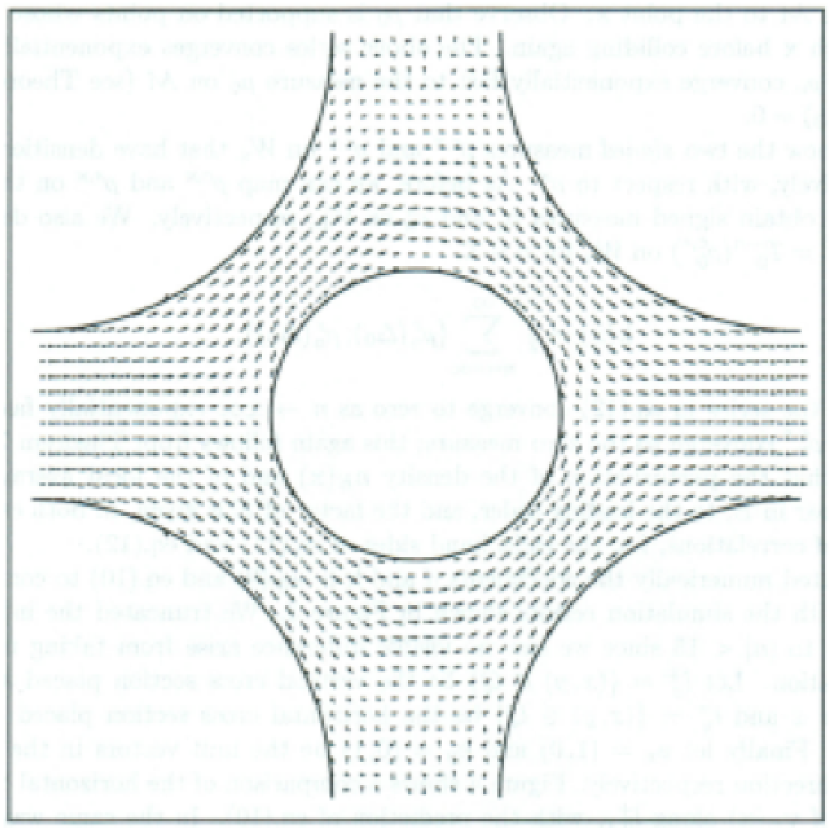
where h_0 is the K-S entropy at zero field and the average current $\mathbf{J}$ is given by

$$\mathbf{J} = \mu_{\mathbf{E}}^{+}(\mathbf{v}) = \underline{\boldsymbol{\sigma}}_0 \mathbf{E} + o(E). \tag{21}$$

Here, $\underline{\boldsymbol{\sigma}}_0$ is the conductivity tensor; it is equal to the diffusion tensor $\underline{\mathbf{D}}$ in zero field, in accord with the Einstein-Green-Kubo relation.

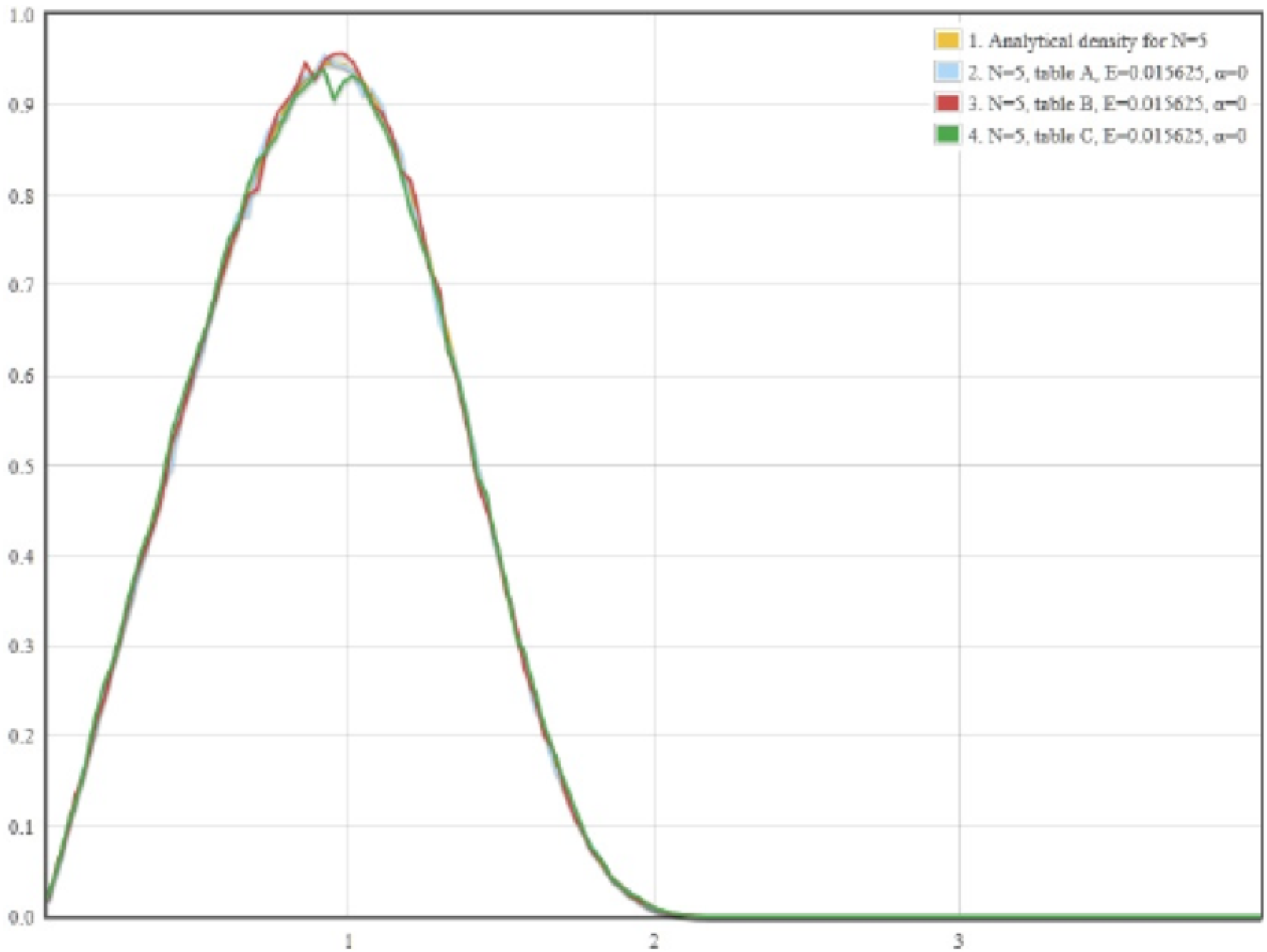
A snapshot of the density of trajectories crossing the Poincaré plane for a very similar model studied by Hoover and Posch. The density would be uniform for $\mathbf{E} = 0$, corresponding to the microcanonical ensemble.

We have also shown recently (Bonetto, Chernov, Korepanov, L.) that despite the singular nature of $\mu_{\mathbf{E}}^{+}$, its projections on space coordinates are absolutely continuous. This is in agreement with results found by Bonetto, Kupiainen, L. about projections of SRB measures. Here is a picture of the flow for table A with the field in the x-direction, $E = 0.1$.



There are no exact results for this system when $N \geq 2$, due to the lack of uniform hyperbolicity in the absence of an external field. Numerical and heuristic results strongly suggest however that this system has a unique NESS for $|\mathbf{E}| \in [0, E_0]$ for all N. This was first noted in Bonetto, Deems, L., Ricci (BDLR) who considered only the geometry in Table A. BDLR also introduced an approximate description in which the obstacles are replaced by random scatterings.

We (Bonetto, Chernov, Korepanov, L.) have recently returned to the study of this system. Surprisingly we find in very high precision numerical simulations that when $|\mathbf{E}|$ is small, say $|\mathbf{E}| \leq .2$, this deterministic mechanical system has a NESS speed distribution which is independent of the shape of the billiard table. In fact, we argue that this speed distribution coincides, in the limit $\mathbf{E} \to 0$, with that obtained from the NESS of a stochastic model which can be computed explicitly, see Figures.


1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
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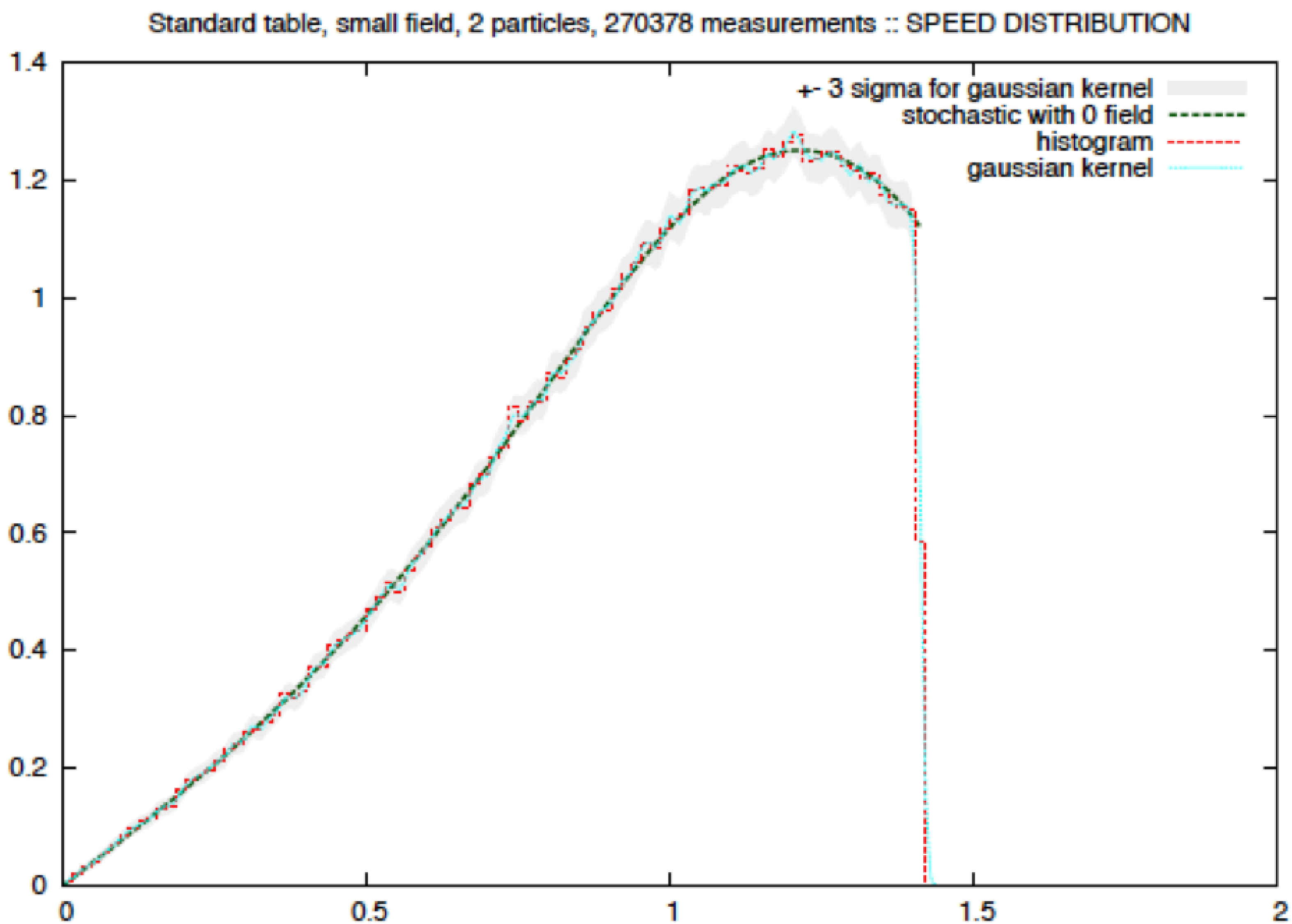
1
2
3
1. Analytical density for N=5
2. N=5, table A, E=0.015625, α=0
3. N=5, table B, E=0.015625, α=0
4. N=5, table C, E=0.015625, α=0


Standard table, small field, 2 particles, 270378 measurements :: SPEED DISTRIBUTION
+- 3 sigma for gaussian kernel
stochastic with 0 field
histogram
gaussian kernel
1.4
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0.8
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0.5
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2

In the stochastic model (designated by S) the equations of motion are the same as (18) **except** that $\mathbf{F}_i$ now represents "random" scatterings by "virtual" collisions which conserve energy but not momentum. More precisely we imagine that each particle will suffer a collision in which the direction of its velocity changes from θ' to θ according to some transition kernel $K(\theta, \theta')\, d\theta$. The exact form of K will turn out not to matter as long as there is enough spreading in the direction of the velocity so that in the absence of a field the collisions will make the angular distribution of the velocity of each particle approach $\frac{d\theta}{2\pi}$.

The scattering “closest” to that caused by collision with fixed discs and the one we used in the simulations is the following: $\mathbf{v}$ changes to $\mathbf{v}'$ according to the rule

$$\mathbf{v}' = \mathbf{v} - 2\hat{\mathbf{n}}(\hat{\mathbf{n}} \cdot \mathbf{v}) \tag{22}$$

where $\hat{\mathbf{n}}$ is a unit vector in the direction of the momentum transfer from $\mathbf{v}$ to $\mathbf{v}'$. The direction of $\hat{\mathbf{n}}$ is random subject to the constraint $(\hat{\mathbf{n}} \cdot \mathbf{v}) < 0$. It corresponds to the ”Boltzmann-Grad limit” of the scatterers with density ρ and diameter a with
$\rho \to 0\,, a \to 0\,, \rho a = l^{-1}$, the inverse of the mean-free path.

The "master" equation describing the time evolution of the N-particle velocity distribution function, which is independent of the positions $\mathbf{q}_i$ is, for the above rule, given by

$$\begin{aligned}\frac{\partial W(\mathbf{V},t)}{\partial t} &= -\sum_{i=1}^{N} \frac{\partial}{\partial \mathbf{v}_i}\Big[\Big(\mathbf{E} - (\mathbf{E}\cdot\mathbf{j})\mathbf{v}_i\Big)W\Big] \\ &\quad + \sum_{i=1}^{N} \frac{1}{2}\int (\mathbf{v}_i' \cdot \hat{\mathbf{n}})\Big[W(\mathbf{V}_i', t; \mathbf{E}) - W(\mathbf{V}, t; \mathbf{E})\Big]\, d\hat{\mathbf{n}} \\ &= E\,\mathcal{B}(W) + \mathcal{C}(W) \end{aligned} \tag{23}$$

where $\mathbf{j} = \mathbf{J}/K$

$$\mathbf{V} = (\mathbf{v}_1, \ldots, \mathbf{v}_i, \ldots, \mathbf{v}_N) \quad \text{and} \quad \mathbf{V}_i' = (\mathbf{v}_1, \ldots, \mathbf{v}_i', \ldots, \mathbf{v}_N), \tag{24}$$

and $\mathbf{v}_i'$ is given in terms of $\mathbf{v}_i$ by (22). In the last term E is the magnitude of $\mathbf{E}$, i.e., $\mathbf{E} = E\mathbf{e}$ for a unit vector $\mathbf{e}$, and $\mathcal{C} = \sum_{i=1}^{N} \mathcal{C}_i$ is the sum of collision terms for the different particles. These occur independently and do not depend on E.

The master (Liouville) equation for the deterministic model would involve also the position coordinates $\mathbf{Q} = (\mathbf{q}_1, \ldots, \mathbf{q}_N)$ and have the form

$$\frac{\partial \tilde{W}(\mathbf{Q}, \mathbf{V}, t)}{\partial t} + \sum_{i=1}^{N} \mathbf{v}_i \frac{\partial \tilde{W}}{\partial \mathbf{q}_i} + \sum_{i=1}^{N} \frac{\partial}{\partial \mathbf{v}_i}\Big[\Big(\mathbf{E} - (\mathbf{E}\cdot\mathbf{j})\mathbf{v}_i\Big)\tilde{W}\Big] = \delta_c W \qquad (25)$$

with $\delta_c W$ representing the collisions with the fixed convex obstacles.

NB: The NESS of the mechanical or of the stochastic model in the limit $\mathbf{E} \to 0$ is not the same as the stationary state for $\mathbf{E} = 0$. In fact for $\mathbf{E} = 0$ there is no interaction between the particles and the energy of each particle remains unchanged in time; it can be prescribed initially in an arbitrary fashion subject only to the condition that $\sum_{i=1}^{N} |\mathbf{v}_i|^2 = N$.

The distribution of speeds would then remain unchanged in time but the collisions (deterministic or stochastic) will randomize its direction.

When E is small the appropriate time scale for the change in the speed of the particles will be, as shown below,of order E^{-2}. On that time scale each particle will have undergone many collisions and so one may then expect to have an autonomous equation for the distribution of the speed.

We write $\widetilde{W}(\mathbf{V},\tau;E) = W(\mathbf{V},tE^{-2};E)$ and observe that it satisfies the rescaled equation

$$\frac{\partial \widetilde{W}(\mathbf{V},\tau)}{\partial \tau} + E^{-1}\mathcal{B}\widetilde{W}(\mathbf{V},t) = E^{-2}\mathcal{C}\widetilde{W}(\mathbf{V},t) \tag{26}$$

We now assume that

$$\widetilde{W}(\mathbf{V},\tau;E) = W^{(0)}(\mathbf{V},\tau) + EW^{(1)}(\mathbf{V},\tau) + E^2W^{(2)}(\mathbf{V},\tau) + O(E^3)$$

This is a very strong assumption, in fact stronger than what we need but it makes the analysis much simpler. We believe that the final result can be justified with a more detailed analysis.

Replacing the above expansion in the equation we get that, for eq.(26) to make sense, we need

$$\mathcal{C}\widetilde{W}^{(0)}(\mathbf{V},\tau) = 0 \tag{27}$$

$$\mathcal{C}\widetilde{W}^{(1)}(\mathbf{V},\tau) = \mathcal{B}\widetilde{W}^{(0)}(\mathbf{V},\tau) \tag{28}$$

$$\frac{\partial\widetilde{W}^{(0)}(\mathbf{V},\tau)}{\partial\tau} + \mathcal{B}\widetilde{W}^{(1)}(\mathbf{V},\tau) = \mathcal{C}\widetilde{W}^{(2)}(\mathbf{V},\tau) \tag{29}$$

Let us set $\mathbf{v}_i = (r_i, \theta_i)$ where $r_i = |\mathbf{v}_i|$ and the angle θ_i is taken with respect to the field direction which we can assume is in the x-direction. We then set $\mathbf{V} = (\mathbf{R}, \mathbf{\Theta})$ and define

$$F(\mathbf{R}, \tau; \mathbf{E}) = \frac{1}{(2\pi)^N} \int \cdots \int \widetilde{W}(\mathbf{R}, \mathbf{\Theta}, \tau/E^2; \mathbf{E})\, d\theta_1 \cdots d\theta_N \equiv \mathcal{E}_{\mathbf{\Theta}} \widetilde{W} \tag{30}$$

Eq.(27) implies that $\widetilde{W}^{(0)}(\mathbf{V},\tau)$ depends only on $\mathbf{R}$. From this it follows that $\mathcal{E}_{\mathbf{\Theta}}\mathcal{B}\widetilde{W}^{(0)}(\mathbf{V},\tau) = 0$ and finally that $W^{(1)}(\mathbf{V},\tau) = \mathcal{C}^{-1}\mathcal{B}\widetilde{W}^{(0)}(\mathbf{V},\tau)$ is well defined. Inserting this expression into eq.(29) and averaging it over $\mathbf{\Theta}$ we get

$$\frac{\partial F^{(0)}(1,\tau)}{\partial \tau} + \mathcal{E}_{\mathbf{\Theta}}\mathcal{B}\mathcal{C}^{-1}\mathcal{B}F^{(0)}(\mathbf{R},\tau) = 0.$$

This equation can be written in the form

$$D^{-1}\frac{\partial F_0(\mathbf{R},\tau)}{\partial \tau} = \sum_{i=1}^{N}\sum_{j=1}^{N}\frac{\partial^2}{\partial r_i \partial r_j}\Big[M_{ij}(\mathbf{R})F_0(\mathbf{R},\tau)\Big] + \sum_{i=1}^{N}\frac{\partial}{\partial r_i}\Big[A_i(\mathbf{R})F_0(\mathbf{R},\tau)\Big] \tag{31}$$

where

$$M_{ij}(\mathbf{R}) = \sum_{k=1}^{N} \frac{b_{ik}(\mathbf{R})b_{jk}(\mathbf{R})}{r_k} = \frac{1}{r_i}\delta_{ij} - \frac{r_i + r_j}{K} + \frac{r_i r_j}{K^2}\sum_{k=1}^{N} r_k \qquad (32)$$

$$A_i(\mathbf{R}) = -\frac{r_i}{K}\sum_{k=1}^{N}\frac{1}{r_k} + \frac{r_i}{K^2}\sum_{k=1}^{N} r_k, \qquad b_{ik} = \delta_{ik} - \frac{r_i r_k}{K} \qquad (33)$$

and D is just the integral of the velocity autocorrelation in the field direction $\mathbf{e}$ when the magnitude of the field $E = 0$. We have $D = \mathbf{e} \cdot \mathbf{D} \cdot \mathbf{e}$, where

$$\mathbf{D} = \frac{1}{|\mathbf{v}_1|}\int_0^\infty \langle \mathbf{v}_1 \otimes \mathbf{v}_1(t) \rangle \; = \frac{1}{|\mathbf{v}_1|}\int_0^\infty \langle \mathbf{v}_1 \otimes e^{\mathcal{C}_1 t}\mathbf{v}_1 \rangle \, dt, \qquad (34)$$

where $\langle \cdot \rangle$ is just averaging with respect to the isotropic measure $d\theta/(2\pi)$ that is stationary for $E = 0$.

D is in fact the only term in (31) which depends on the collision kernel $\mathcal{C}$ in (23). For the isotropic scattering considered so far

$$D = \frac{1}{2\pi}\int_0^{2\pi} d\theta \int_0^{\infty} [cos\theta \cos\theta(t)]\, dt. \tag{35}$$

For the specific model used in (23), $D = 3/4$.

In the case of billiards D will depend on the shape of the table. Note however that the NESS corresponding to the stationary solution of (31) is independent of D which really just sets a time scale.

We note that

$$M = SS^* \qquad \text{with} \qquad S_{ij}(\mathbf{R}) = \frac{b_{ij}(\mathbf{R})}{\sqrt{r_j}} \tag{36}$$

which means that (31) corresponds to a stochastic evolution described by the Itô stochastic differential equation

$$\frac{dr_i}{dt} = \sqrt{D}\Big[A_i(\mathbf{R}) + \sum_{j=1}^{N} S_{ij}(\mathbf{R})\,\frac{dB_j}{dt}\Big]. \tag{37}$$

One can in fact first derive (37) and then obtain (31). Using some general theory this shows that the solution of (31) is unique.

The stationary solution of (31), $\bar{F}_0$, which is in fact the limit as $t \to \infty$ of $F_0(\mathbf{R}, t)$, is independent of D, and is given, when the initial state is such that $K = N$, by

$$\bar{F}_0(\mathbf{R}) = \frac{1}{Z} \delta(K - N) \left[\sum_{i=1}^{N} r_i^3 \right]^{-\frac{2N-1}{3}} \tag{38}$$

where Z is just the normalization

$$Z = \int_{\sum r_i^2 = N} \left[\sum_{i=1}^{N} r_i^3 \right]^{-\frac{2N-1}{3}} \prod_{i=1}^{N} r_i \, dr_i \tag{39}$$

To get the one particle marginal speed distribution $f_0(r; N)$ one has to integrate (38) over the variables $r_2, \ldots, r_N$.

Going beyond the limit $E \to 0$ we find the first order correction (in E) to the stationary solution of (31):

$$W(\mathbf{R},\mathbf{\Theta};E,N) = F_0(\mathbf{R}) + EF_1(\mathbf{R},\mathbf{\Theta}) + o(E), \tag{40}$$

where

$$F_1(\mathbf{R},\mathbf{\Theta};N) = (2N-1)\left[\sum_{i=1}^{N} r_i^3\right]^{-\frac{2N+2}{3}} \sum_{i=1}^{N} r_i c(\theta_i) \tag{41}$$

and

$$c(\theta_i) = \mathcal{C}_i^{-1} \cos\theta_i \tag{42}$$

and $\mathcal{C}_i$ is the collision operator defined on the right hand side of (23). Note that $\mathcal{C}_i$ is independent of N so the linear term in E is simply related to that of the $N = 1$ problem. This is checked via simulations.

Large N limit

This universality of $E \to 0$ becomes even more striking when $N \to \infty$. In this limit the one particle speed distribution $f_{\mathbf{E}}(v, N) \to \tilde{f}_{\mathbf{E}}(v)$ as $N \to \infty$, given by

$$\lim_{\mathbf{E} \to 0} \tilde{f}_{\mathbf{E}}(v) = \tilde{f}_0(v) = Cve^{-cv^3}, \quad v = |\mathbf{v}| \tag{43}$$

where

$$C = \frac{\sqrt{3}}{3} \frac{1}{\Gamma\left(\frac{2}{3}\right)^3} \approx 0.233, \tag{44}$$

$$c = \frac{2}{27} \frac{\sqrt{2}\pi^{\frac{3}{2}} 3^{\frac{3}{4}}}{\Gamma\left(\frac{2}{3}\right)^3} \approx 0.536 \tag{45}$$

are determined uniquely by the requirements that

$$\int_0^\infty v^2 \tilde{f}_0(v)\, dv = \int_0^\infty \tilde{f}_0(v)\, dv = \frac{1}{2\pi}. \tag{46}$$

We find numerically that (43) holds with high precision for both the mechanical and stochastic systems. It is also the solution of the self-consistent Boltzmann equation discussed later.

(The distribution (43) can also be related to the time rescaled ($v/t^{1/3}$) distribution of a single particle in a field E without thermostat, studied by Chernov and Dolgopyat.)

Large field

When the field is large, the mechanical system behaves very differently from the stochastic one, with particle trajectories essentially “hugging” the obstacles. The stochastic one is of course always spatially uniform.

On the other hand we also find (numerically) that for $N >> 1$ the one-particle marginal velocity distribution of the stochastic model is very close to that obtained from the solution of a self-consistent Boltzmann equation introduced in BDLR. This can actually be proven in the limit $N \to \infty$ (work in progress with Bonetto, Carlen, Esposito and Marra).

Self-consistent BE

A heuristic derivation of the BE from eq.(18) with F_i stochastic is based on the intuitive idea that, $\mathbf{j} = \sum_{i=1}^{N} \mathbf{v}_i/N$, in eq.(18) will approach, in the limit $N \to \infty$, a deterministic value $\langle \mathbf{v} \rangle$. This yields then an equation for the one particle marginal

$$\frac{\partial}{\partial t} f(\mathbf{v},t) + \frac{\partial}{\partial \mathbf{v}} \left[\left(\mathbf{E} - \frac{\mathbf{E} \cdot \langle \mathbf{v} \rangle}{\langle |\mathbf{v}|^2 \rangle} \mathbf{v} \right) f(\mathbf{v},t) \right] = \frac{1}{l} \int_{\mathbf{v}\cdot\mathbf{n}<0} \frac{\mathbf{v}' \cdot \mathbf{n}}{2} \Big(f(\mathbf{v}',t) - f(\mathbf{v},t) \Big) \, d\mathbf{n} \tag{47}$$

Eq.(47) yields immediately that

$$\frac{d}{dt} \int |\mathbf{v}|^2 f(\mathbf{v},t) \, d\mathbf{v} = \frac{d}{dt} \, \langle |\mathbf{v}|^2 \rangle = 0 \tag{48}$$

so that if we chose $f(\mathbf{v},0)$ such that $\langle |\mathbf{v}(0)|^2 \rangle = 1$ we will have $\langle |\mathbf{v}(t)|^2 \rangle = 1$ for all t. The current $\langle \mathbf{v}(t) \rangle = \mathbf{j}$ will then have to be determined self-consistently from the solution of the BE.

Quantum Systems Coupled to Thermal Reservoirs

The "Markovian idealization" used for classical systems is no longer so simple for quantum ones, and it is far from obvious how to write down a Markovian equation for the density matrix, ρ, of a system coupled to reservoirs which is analogous to the classical case, i.e. we look for an equation of the form

$$\frac{\partial \rho_t}{\partial t} = \frac{1}{i}\,[H, \rho_t] + \widehat{\mathcal{K}}\rho_t = L\rho_t.$$

In addition to the obvious requirement that L preserve normalization and positivity of ρ, there is the Lindblad complete positivity condition on the "Markovian" operator $\widehat{\mathcal{K}}$.

Complete positivity ensures positivity of the joint density matrix of our system and another independent system which does not interact with any reservoirs. This is clearly a necessary condition for ρ_t which is not automatically satisfied by positivity of ρ_t. This is different from the classical case and puts restrictions on the kind of Pauli master equation we can have for a density matrix. In a very interesting paper, Castella, Erdos, Frommlet, and Markovich corrected the results of a famous paper by Caldeira and Leggett who derived a master equation for a particle moving in a harmonic potential and linearly coupled to a heat bath of quantum oscillators which did not have the Lindblad form.

Lindblad Stochastic Evolution

$$\widehat{\mathcal{K}}\rho = \frac{1}{2}\sum_{i,j} C_{ij}\left\{\left[F_i, \rho F_j^\dagger\right] + \left[F_i\rho, F_j^\dagger\right]\right\}$$

The F_ℓ are operators on the system's finite N-dimensional Hilbert space, $tr\left(F_i^\dagger F_j\right) = \delta_{ij}$, and $\left\{C_{ij}\right\}$ is a positive (semi-definite) matrix. This is a necessary and sufficient condition for the time evolved density matrix $\rho(t)$ to have the "Kraus form" of a completely positive map

$$\rho_t = \sum_{i=1}^{k} A_i(t)\rho_0 A_i^\dagger(t)$$

with

$$\sum_{i=1}^{k} A_i A_i^\dagger = 1.$$

How do we get such a $\widehat{\mathcal{K}}$? Start with an interacting system-reservoir Hamiltonian,

$$H_\lambda = H_S \otimes 1^R + 1^S \otimes H^R + \lambda H^{SR}$$

$$H^R = H_1^R + \cdots H_r^R, \quad \text{infinite reservoirs}$$

Let W_t be the joint system-reservoir density matrix

$$W_t = U_t^\lambda W_0 = e^{-iH_\lambda t} W_0 e^{iH_\lambda t}.$$

Assume that at $t = 0$, $W_0 = \rho_0 \otimes \omega^R$ where

$$\omega^R = \omega^1 \otimes \cdots \otimes \omega^r$$

$\omega^{(i)}$ KMS (Gibbs) states at inverse temperature β_i. Then

$$\begin{aligned} \rho_t &= Tr_R \left[U_t^\lambda \left(\rho_0 \otimes \omega^R \right) \right] \\ &= \Lambda_t^\lambda \rho_0 \end{aligned}$$

which will automatically be of the Kraus form. Then we can write

$$\frac{\partial \rho_t}{\partial t} = \frac{1}{i} \left[H_S, \rho_t \right] + \lambda^2 \int_0^t ds K_\lambda(t-s) \rho_s$$

and K_λ has a power series expansion in λ.

It was proven by Davies that under suitable conditions on the reservoirs and interactions V^{SR}, one can carry out the van Hove limit,

$$\lambda \to 0,\ t \to \infty,\ \lambda^2 t \to \tau,$$

and obtain a Markovian equation for the density matrix of the system, ρ_τ,

$$\frac{\partial \rho_\tau}{\partial \tau} = L\rho_\tau = \frac{1}{i}\left[H_S, \rho_\tau\right] + \widehat{\mathcal{K}}\rho_\tau,$$

where $\widehat{\mathcal{K}} = \int_0^\infty ds K_0(s)$ is of the Lindblad form.

The essential requirement for this to hold is that the reservoir correlations decay sufficiently rapidly, e.g. if $V^{\mathrm{SR}} = V^S \otimes V^R$ and the reservoirs are ideal Fermi gasses then

$$\left| tr_R \left(\omega_R V^R(t) V^R(0) \right) \right| < a(1+t)^{-(1+\epsilon)}.$$

Going Beyond the van Hove Limit

There is much work in this area by many people including, in particular, Erdos, Jaksic, Pillet, Yau, and collaborators. Let me just mention a few recent results.

Let

$$\rho_\tau = e^{L\tau}\rho_0 = \Lambda^0_\tau \rho_0$$

be the solution of the Markovian equation. Then one can show (under suitable assumptions) that $\lim_{\tau\to\infty}\rho_\tau = \rho_{\mathrm{st}}$ is a stationary state, $\rho_{\mathrm{st}} = e^{L\tau}\rho_{\mathrm{st}}$. In particular, if all the reservoirs have the same temperature β^{-1}, then $\rho_{\mathrm{st}} = Z^{-1}e^{-\beta H_S}$.

Consider now

$$\rho^\lambda_{\mathrm{st}} = \lim_{t\to\infty}\Lambda^\lambda_t \rho_0.$$

Froehlich et al., DeRoeck and Kupianen prove for (a single, free reservoir) small λ (and other technicalities) that this limit exists.

Furthermore,

$$\rho_{\mathrm{st}}^{\lambda} \longrightarrow \widehat{\rho}_{\mathrm{st}} \;\text{ as }\; \lambda \to 0,$$

e.g. for a single temperature β^{-1}

$$\rho_{\mathrm{st}}^{\lambda} = Tr_R \left[\exp - \beta \left(H_0 + H^R + \lambda H^{SR} \right) \right] / Z.$$

By the way, even in the case of several reservoirs, the stationary density matrix for $\lambda \to 0$, ρ_{st}, will be a function of H_S. We have to go to the next order in λ to see a truly "heat conducting" stationary state.

On the other hand one can actually obtain the lowest order, $\mathcal{O}(\lambda^3)$ term in the stationary heat current by considering the rate of change of the (left) reservoir energy, as computed from $\widehat{\rho}_{st}$.