Hőegyenlet newtoni mechanikából?

Szász Domokos
(BME Matematika Intézet, Sztochasztika Tsz.)

Alkalmazott Matematikai Nap
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J. von Neumann: ”The Mathematician” (1947)

”Ha egy matematikai diszciplína messzire távolodik tapasztalati forrásától, az súlyos veszélyeket rejt magában. A forrásától eltávolodott folyó jelentéktelen ágak sokaságává különül el és a diszciplína részletek és bonyodalmak szervezetlen tömegévé válik.” (in The Works of the Mind (1947))

D. Szász: *John von Neumann, the Mathematician*,
THE MATHEMATICAL INTELLIGENCER, **33**, No 2 (2011), 42-51

Contents

Heat Equation (no mass flow)

$$\frac{\partial T(x,t)}{\partial t} = \frac{1}{c}\nabla\left[\kappa\nabla T(x,t)\right]$$

c - specific heat/unit volume $(= 1)$
$\kappa = \kappa(T)$ - thermal conductivity

For a wide class of models: $\kappa(T) = \mathrm{const.}\sqrt{T}$
(insulating materials, or gas of weakly/rarely interacting particles)

However: de Roeck-IP Tóth: (in progress)

$$\kappa(T) = \frac{\mathrm{const.}}{T^{3/2}}$$

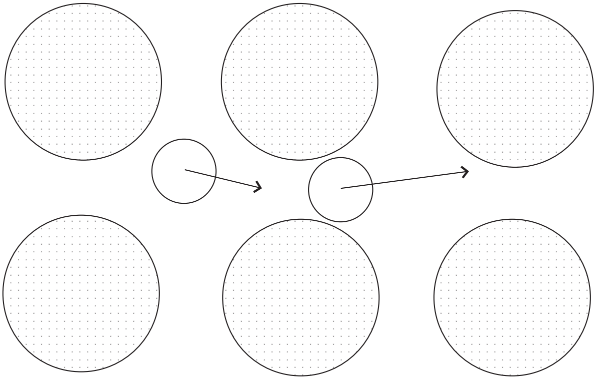
Oscillating interest since late 60's. Some surveys:

1. **Bonetto-Lebowitz-Rey-Bellet** in Math. Phys 2000, Imp. Coll.
2. **Dhar** in Adv. Phys, 2008, 1-78.

Recent wave:

- Ruelle, CMP, 1996 - Dolgopyat, Inv. Math, 2004: Linear response theory vs. differentiability of SRB states
- **Eckmann-Young, CMP, 2006** (also Lin-Young, 2010) non-equilibrium steady states under phenomenological assumptions
  (Krámli-Simányi-Sz., JSP, 1987: RWwIS, temperature profile by postulating local equilibrium)
- **Gaspard-Gilbert, PhRL, 2008–:** model of localized hard disks (balls) - a two step approach:
  1. - derive a mesoscopic master equ. from the microscopic kinetic equ. of the Hamiltonian model
     - in the rare (but strong) interaction limit
     - it is a Markov jump process
  2. derive the macroscopic heat equ. from the mesoscopic master equ.

No mass transport (Coquard et al., J. Non-Crystalline Solids, 2013:
Modelling of conductive heat transfer
though nano-structured porous silica materials)



Parameter choice of Gaspard-Gilbert,'08.

- box size: *1*; periodic b. c.'s along y-axis
- chain length $= N$;
- radius of fixed scatterers (shaded circles)$= \rho_f$
- radius of moving disks (empty circles) $= \rho_m$
- condition of **confinement**: $\rho_f + \rho_m > 1/2$
- condition of **conductivity**:
  $\rho_m > \rho_{crit} = \sqrt{(\rho_f + \rho_m)^2 - (1/2)^2}$
- small parameter $\varepsilon = \rho_m - \rho_{crit} > 0$

Gaspard-Gilbert's trick:

- Keep $\rho_f + \rho_m =: \rho$ fixed
- If $\rho_m = \rho_{crit}$, then we have N non-interacting billiards.
  Moreover, their phase spaces only depend on ρ!

Liouville equation

Ernst-Dorfman, '89: The kinetic equ. for the N-particle density $p_N(q_1, v_1, \ldots, q_N, v_N; t)$ is

$$\partial_t p_N = \sum_{j=1}^{N} \left(-v_j \partial_{q_j} + K_{wall,j} + C_{j,j+1}\right) p_N$$

- the first two terms on the RHS describe the billiard dynamics of each disk within its cell (denote wall collision rate by $\nu_{\mathrm{wall},\varepsilon}$)
- the third one: the interaction of neighboring disks provides the energy transfer (denote binary collision rate by $\nu_{\mathrm{bin},\varepsilon}$)

Scale separation

Gaspard-Gilbert '08. '09: Scale separation at

$\varepsilon \searrow 0$, i. e. $\nu_{\mathrm{wall},\varepsilon} (\sim \nu_{wall,crit} > 0) \gg \nu_{\mathrm{bin},\varepsilon} \to 0$

1. **they derive a master equation for the density** $P_N(E_1, \ldots, E_N; t)$ **(**$E_j = v_j^2 : 1 \leq j \leq N$**)**
2. HDL: **from the master equation they obtain the coefficient of heat conductivity**: $\kappa = \mathrm{const.}\sqrt{T}$ (??, but Sasada, ms in progress)

2011, Cuernavaca: Derivation of diffusion/superdiffusion for mechanical models. Henryk Larralde: Why?
2013, B. Fernandez: True understanding

2011, S. Olla: GG's derivation of HDL uses an incorrect symmetry argument
2013, M. Sasada: correction, based on Green-Kubo (still heuristic)

Challenge: Rigorous theory for GG

Keller-Liverani, CMP, 2009: rare interaction limit.
CML, i. e. interval maps **coupled by collisions**. Result: Uniqueness of SRB and exponential space-time corr. decay.

Dolgopyat-Liverani, CMP, 2011: weak interaction limit.
Mesoscopic equ. is a system of interacting stochastic differential equ.'s.

Dolgopyat-Nándori (in progress): Heat equ. from deterministic dynamics BUT with stochastic bry conditions corresponding to different temperatures

Li Yau-LS Young (in progress): stochastic dynamics in slab w. different bry temperatures. Task: definition of local temperature!?

Dynamical approach for step 1

By Hirata-Saussol-Vaienti, CMP, 1999 (also Collet-Eckmann, Springer, 2006; Chazottes-Collet, EThDS, 2013): *If*

- *a dynamical system* (M, T, μ) *is mixing in a controlled way (e. g.* α*-mixing)*
- *and* A_ε *is a sequence of nice subsets (to avoid e. g. neighborhoods of periodic points) with* $\lim_{\varepsilon\to 0}\mu(A_\varepsilon) = 0$

then the **successive entrance times of the dynamics into** A_ε **form a Poisson process on the time scale of** $\mu(A_\varepsilon)^{-1}$.

For simplicity let $N = 2$ with free boundary conditions along x-axis. The model is isomorphic to a 4D semi-dispersing billiard. It is K-mixing, but no mixing rate is known. (Bálint-Tóth, '08 is for dispersing billiards, only, and, moreover, it is hypothetical).

Conjecture for 2-disk chain, with IP Tóth

$N = 2$, free boundary along x-axis. Dynamics: $(\varepsilon = \rho_m - \rho_{crit})$ $(M_\varepsilon = \{q_1, v_1; q_2, v_2 | dist(q_1, q_2) \geq 2\rho_m, v_1^2 + v_2^2 = 1\}), S^{\mathbb{R}}, \mu_\varepsilon)$. Denote by $0 < \tau_{1,\varepsilon} < \tau_{2,\varepsilon} < \dots$ successive binary collision times of the two disks. Then, as $\varepsilon \to 0$

- $E_1(\nu_{\mathrm{bin},\varepsilon} t), E_2(\nu_{\mathrm{bin},\varepsilon} t)$ converges to a jump Markov process on the state space $E_1 + E_2 = 1$ where $E_j(t) = \frac{1}{2} v_j^2(t); j = 1, 2$
- the transition kernel $k(E_1^+ | E_1^-)$ is calculated by verifying Boltzmann's 'microscopic chaos' property (cf. scattering cross section)

Note: $\nu_{\mathrm{bin},\varepsilon} \sim \mathrm{const}.\varepsilon^3$.

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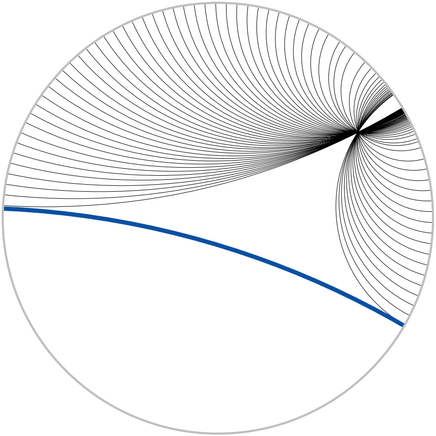
Envisioned proof

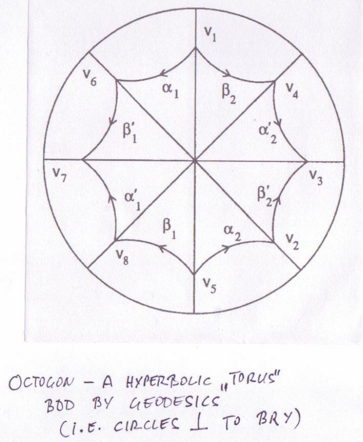
- since binary collisions are rare, most of the time the two disks evolve independently
- between two binary collisions - with an overwhelming probability - there is averaging in each of the in-cell, 2D billiard dynamics
- for these typically long time intervals it is natural to apply Chernov-Dolgopyat averaging
- for that purpose
  - one checks that for an incoming proper family of stable pairs, so is the outgoing family ???
  - one applies martingale approximation for jump processes (á la Ethier-Kurtz)

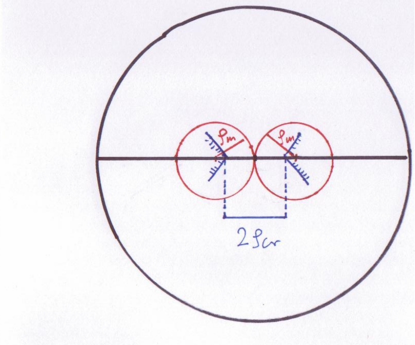
Paradigm: in-cell dynamics is billiard in cpct constant negative curvature

P Bálint-P Nándori-D. Sz.-T. Tasnády-IP Tóth; in progress
Geodesics in Poincaré model of hyperbolic geometry



Hyperbolic "octagonal tori"





Phase space: dim $M = 7$. Scatterers 16 boundaries, + 1 "cylinder"

Goal: Mimic the geometry of GG model.

Warm-up result

P Bálint-P Nándori-D. Sz.-T. Tasnády-IP Tóth, 2013

For a reasonable set of $0 < \rho_{cr} < \rho_m$ the billiard model is ergodic and K-mixing. Tools:

- **(un)stable invariant manifolds of the billiard in the octagon with rectangular geodesic edges are (un)stable invariant manifolds of the non-compact model reflected through the edges of the octagon**
- Chernov-Sinai, 1987 type local ergodicity theorem in the form of Liverani-Wojtkowski, 1995
- Krámli-Simányi-Sz., 1989: method for semi-dispersing billiards

Second fundamental form of the superficies

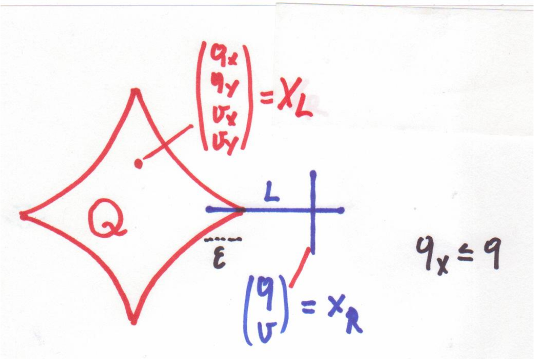
Skew cylinder: superficies set (i. e. generator in Euclidean geometry): $A = \{(x, y) | d(x, y) = 2\rho_m\}$
Notation:
$\mathbf{n}$ = collision unit normal pointing to the right
$\mathbf{t}$ = collision unit tangent ($\mathbf{n}$ rotated with angle $\pi/2$)
Local orthogonal "basis":

$$N = \begin{pmatrix} -\mathbf{n} \\ \mathbf{n} \end{pmatrix} \quad T_1 = \begin{pmatrix} \mathbf{n} \\ \mathbf{n} \end{pmatrix} \quad T_2 = \begin{pmatrix} \mathbf{t} \\ \mathbf{t} \end{pmatrix} \quad T_3 = \begin{pmatrix} \mathbf{t} \\ -\mathbf{t} \end{pmatrix}$$

Eigenvalues: $0, \tanh \rho_m, \coth \rho_m$

Dimension reduction: Billiard coupled to a piston

Collision rule: $v_x^+ = v^-, v^+ = v_x^-, v_y^+ = v_y^-$.



$$(q_x, q_y) \in Q,$$
$$q \in [-\varepsilon, L - \varepsilon]$$

Transition kernel

$$k(E_L'|E_L) \sim \varepsilon^2 \frac{\tan\beta}{2\pi L|Q|} \frac{\sqrt{1-\min\{E_L, E_L'\}}}{\sqrt{1-E_L'}\sqrt{E_L+E_L'-1}} \mathbb{1}_{\{E_L+E_L'>1\}}$$

thus for the rate $\Lambda(E_L) = \int_0^1 k(e|E_L)de$ one has $\varepsilon^{-2}\Lambda(E_L) =$

$$= \begin{cases} \frac{\tan\beta}{L|Q|}\sqrt{1-E_L} & \text{if } E_L < 1/2, \\ \frac{\tan\beta}{L|Q|}\left[\sqrt{2E_L-1} + \frac{\sqrt{1-E_L}}{2}\left(\frac{\pi}{2} - \arcsin\left(3 - \frac{2}{E_L}\right)\right)\right] & \text{if } E_L \geq 1/2. \end{cases}$$

Step 2: A (mesoscopic) stochastic model of energies

Grigo-Khanin-Sz. Nonlinearity, 2012.

State space: $x = (x_1, \ldots, x_N) \in \mathbb{R}_+^N$

Generator $\mathcal{L}$ of the continuous time Markov jump process $X(t)$ (given on $\mathbb{R}_+^N$) acting on bounded functions $A : \mathbb{R}_+^N \to \mathbb{R}$ is

$$\mathcal{L}A(x) = \sum_{i=1}^{N-1} \Lambda(x_i, x_{i+1}) \int P(x_i, x_{i+1}; d\alpha) \left[A(T_{i,\alpha}x) - A(x)\right]$$

where $P(x_i, x_{i+1}; d\alpha)$ is a probability measure on $[0, 1]$.

The maps $T_{i,\alpha}$, modelling energy exchange between the neighboring sites i and $i+1$, are defined by

$$T_{i,\alpha}(x_i) = \alpha(x_i + x_{i+1})$$

$$T_{i,\alpha}(x_{i+1}) = (1-\alpha)(x_i + x_{i+1})$$

Remarks

- Total energy is invariant, i. e.

$$\mathcal{S}_{\epsilon,N} = \left\{ x \in \mathbb{R}_+^N \middle| \sum_{i=1}^{N} \frac{1}{N} x_i = \epsilon \right\}$$

  is invariant wrt dynamics;

- Standing assumptions:
  1. for any E, E', the kernel $P(E, E', d\alpha)$
     1. is symmetric wrt $1/2$;
     2. is never equal to $\frac{1}{2}(\delta_0 + \delta_1)$ (i. e. $\{E_1^+, E_2^+\} \neq \{E_1, E_2\}$)
  2. plus an appropriate condition for Λ.

Mesoscopic generator in the GG model, case $d = 3$

$$\Lambda(E_1, E_2) = \Lambda_s(E_1 + E_2)\ \Lambda_r\left(\frac{E_1}{E_1 + E_2}\right)$$

(factorization property!) where

$$\underline{\Lambda_s(s) = \sqrt{s}} \qquad\qquad \Lambda_r(\beta) = \frac{2\pi}{6}\ \frac{\frac{1}{2} + \beta \vee (1-\beta)}{\sqrt{\beta \vee (1-\beta)}}$$

and

$$P(x_1, x_2; d\alpha) = P\left(\frac{x_1}{x_1 + x_2}; d\alpha\right) = P(\beta; d\alpha)$$

with $\beta = \frac{x_1}{x_1+x_2}$ (simple dependence!), where

$$\frac{P(\beta; d\alpha)}{d\alpha} = \frac{3}{2}\ \frac{1 \wedge \sqrt{\frac{\alpha\wedge(1-\alpha)}{\beta\wedge(1-\beta)}}}{\frac{1}{2} + \beta \vee (1-\beta)}.$$

Limiting heat equ. in GG model

In the limit, as $N \to \infty$ and $\xi = i/N$, $t = N^2 \tau$, the empirical process

$$\sum_{i=1}^{N} \frac{1}{N} \delta_{X_i(t)}$$

should converge to a process with density $T(x,t)$ solving

$$\frac{\partial T(x,t)}{\partial t} = \mathrm{const.} \nabla \left[\sqrt{T(x,t)} \nabla T(x,t) \right]$$

Main result for GG

Theorem (G-Kh-Sz, 12)

If $\Lambda_s(s)$ is replaced by any non-negative continuous function, which is bounded away from zero, then, for any N and ϵ,

1. *For $d \geq 2$,*
   1. *The product measure $\mu(dx) = \nu(dx_1) \cdots \nu(dx_N)$ with $\nu(dx_1) = \Gamma(\frac{d}{2} - 1)$ is the unique non-degenerate reversible product measure for $X(t)$.*
   2. *On every $\mathcal{S}_{\epsilon,N}$ there exists a unique stationary distribution $\pi_{\epsilon,N}$. This measure is obtained by conditioning $\mu(dx)$.*
2. *For $d \geq 3$, the spectrum $\sigma(\mathcal{L})$ of the generator $\mathcal{L}$ acting on $L^2_{\pi_{\epsilon,N}}$ satisfies*

$$\sigma(\mathcal{L}) \subset \Big(-\infty, -C \sin^2 \Big[\frac{\pi}{N+2}\Big]\Big] \cup \{0\}$$

for some constant C, which may depend on the choice of Λ_s.

Sasada's gap bd, invited talk at ICMP12

Assume that the rate function Λ factorizes and satisfies $\Lambda(a,b) \geq \Lambda^*(a+b)^m$ for some $\Lambda^* > 0$ and $m \geq 0$. (cf. porous medium equ.)
Denote the spectral gap for the N-chain by $\gamma^{(m)}(\varepsilon, N)$ wrt reversible measure $\bigotimes_1^N \Gamma(g)$ conditioned to $\mathcal{S}_{\epsilon,N}$ ($g = \frac{d}{2} - 1$ from before).

Theorem (Sasada: arXiv:1305.4066)

There exists a positive constant C depending only on Λ^*, m and g such that $\forall \varepsilon > 0$ and $N \geq 2$

$$\gamma^{(m)}(\varepsilon, N) \geq C\varepsilon^m \frac{1}{N^2}.$$

Cf. Kac' model for heat exchange and Boltzmann equation

THANKS