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Mixing in a model of heat conduction

Domokos Szász Budapest University of Technology (joint with Alex Grigo and Kostya Khanin)

Ergodic Theory and Dynamical Systems: Perspectives and Prospects

Warwick, April 17, 2012

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 Intro: Gaspard-Gilbert's two-step approach to derivation of heat equ.

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- 2 A deterministic model of heat conduction
- **3** Dynamical approach to Step 1
- Mesoscopic stochastic models of energies for Step 2
- **6** Lower bound for spectral gap of generators
- 6 Reversible product measures
- Derivation of the heat equation

Non-equilibrium statistical physics

Goal: macroscopic laws from microscopic dynamics. Optimally: from Newtonian (Hamiltonian) ones (classical statphys!)

Strong candidates:

- billiard models (quite realistic)
- (non-linear) oscillators

Spectacular successes for billiards:

- planar diffusion (or super-diffusion); Bunimovich, Chernov, Sinai '81, '91; Young '98; Sz.-Varjú '04, '07; Bálint-Gouëzel '06; Chernov-Dolgopyat 09 — , Rey-Bellet-Young '08, Melbourne-Nicol '09, Gouëzel '10, etc., etc.
- linear Boltzmann equation for the Lorentz gas (Boldrighini, Bunimovich, Sinai, '83)
- convergence to equilibrium of Lorentz gas (Krámli-Sz., '83)

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Derivation of heat equ. Fourier law of heat conduction

Oscillating interest:

survey until 2000: Bonetto-Lebowitz-Rey-Bellet '00 Recent wave:

- Eckmann-Young '06: equilibrium measures under phenomenological assumptions
- Gaspard-Gilbert '08-: model of localized hard disks (balls), 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. $\partial_t u = \partial_x(\kappa(u)\partial_x u)$ from the mesoscopic master equ.

• and determine $\kappa(u)$



Periodic scatterers (shaded disks), confined moving disks (white circles)



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Parameter choice of G-G,'08.

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

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• small parameter $\varepsilon = \rho_m - \rho_{crit}$

G-G'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 !

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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 ν_{wall,ε})

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• the third one: the interaction of neighboring disks provides energy transfer (denote binary collision rate by $\nu_{\text{bin},\varepsilon}$)

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Scale separation

G-G '08-: Scale separation at

 $\varepsilon
ightarrow 0$, i. e. $u_{\mathrm{wall},\varepsilon}(\sim
u_{\mathit{wall},\mathit{crit}} > 0) \gg
u_{\mathrm{bin},\varepsilon}
ightarrow 0$

• they derive a master equation for the density $P_N(E_1, ..., E_N; t)$ $(E_j = v_j^2 : 1 \le j \le N)$

Provide the master equation they obtain the coefficient of heat conductivity: κ(T) = √T (T being the temperature)
 i. e. the equation ∂_tu = C . Δu^{3/2}.

Our aim: Rigorous theory

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Dynamical approach to step 1

By Hirata-Saussol-Vaienti, '98 (also Collet-Eckmann, '06, Chazotte-Collet '10): *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_{ε→0} μ(A_ε) = 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. (exponential mixing: Bálint-Tóth, '08 is for dispersing billiards, only, and, moreover, it is hypothetical).

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similarly for N-disks, too

(joint with IP Tóth, work in slow progress) N = 2, free boundary condition along x-axis. Dynamics: $(M_{\varepsilon} = \{q_1, v_1; q_2, v_2 | dist(q_1, q_2) \ge 2\rho_m, v_1^2 + v_2^2 = 1\}, S^{\mathbb{R}}, \mu_{\varepsilon}).$ Denote by $0 < \tau_{1,\varepsilon} < \tau_{2,\varepsilon} < \ldots$ successive binary collision times of the two disks. Then, as $\varepsilon \to 0$

- $(\nu_{\mathrm{bin},\varepsilon}\tau_{1,\varepsilon},\nu_{\mathrm{bin},\varepsilon}\tau_{2,\varepsilon},\dots)$ converges to a Poisson process
- $E_1(\nu_{\text{bin},\varepsilon}t), E_2(\nu_{\text{bin},\varepsilon}t)$ 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(E₁⁺|E₁⁻) is calculated by verifying Boltzmann's 'microscopic chaos' property

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

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Idea of 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 has to check that for an incoming proper family of stable pairs, so is the outgoing family ???
 - one applies martingale approximation for jump processes (á la Dolgopyat-Sz.-Varjú, Duke '09)



Our approach (with Grigo and Khanin)

- Introduce a (mesoscopic) stochastic model close to that of GG;
- Find lower bounds for the spectral gap of its generator (appropriately depending on system size N).
- **③** Establish hydrodynamics limit transition to obtain heat equ.

Appropriate dependence = $O(\frac{1}{N^2})$ for continuous time dynamics.

Existing gap bounds almost exclusively for models with a finite state-space (like exclusion-like processes).

Continuous state space model: for Kac-model from '56 spectral gap estimate by Janvresse in '01, only.

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A (mesoscopic) stochastic model of energies

State space: $x = (x_1, ..., x_N) \in \mathbb{R}^N_+$ 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 $T_{i,\alpha}$ model the energy exchange between the neighboring sites *i* and *i* + 1, and are defined by

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

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Remarks

• Total energy is invariant, i. e.

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

is invariant wrt dynamics;

Standing assumptions: for any E, E' the kernel P(E, E', dα)
is symmetric wrt 1/2;
is never equal to ½(δ₀ + δ₁) (i. e. {E₁⁺, E₂⁺} ≠ {E₁, E₂})
plus an appropriate condition for Λ.

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Mesoscopic generator in the GG model, case d = 3

$$\Lambda(E_1, E_2) = \Lambda_{tot}(E_1 + E_2) \Lambda_{part}(\frac{E_1}{E_1 + E_2})$$

(product!) where

$$\Lambda_{tot}(s) = \sqrt{s} \qquad \qquad \Lambda_{part}(\beta) = \frac{2\pi}{6} \ \frac{\frac{1}{2} + \beta \vee (1 - \beta)}{\sqrt{\beta \vee (1 - \beta)}}$$

and

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

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

$$rac{P(eta, dlpha)}{dlpha} = rac{3}{2} \, rac{1 \wedge \sqrt{rac{lpha \wedge (1-lpha)}{eta \wedge (1-eta)}}}{rac{1}{rac{1}{2} + eta ee (1-eta)}}.$$

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Feng-Iscoe-Seppalainen, '96

$$\mathcal{K}A(x) = \sum_{i=1}^{N-1} \frac{1}{2} \int_0^{x_i} u^{\alpha-2} \left(\sum_{j=\pm 1} [A(x^{u,i,j}) - A(x)] \right) du$$

where $\alpha > 1$ and

$$x_k^{u,i,j} = \begin{cases} x_k & \text{if } k \neq i, i+j \\ x_i - u & \text{if } k = i \\ x_{i+j} + u & \text{if } k = i+j \end{cases}$$

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This model can be understood as a zero-range energy model Then the expected limiting equ. is $\partial_t u = \text{const.} \Delta(u^{\alpha})$, the nonlinear heat equ. (porous medium equ.) if $\alpha \neq 1$.

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Goal: Limiting heat equ. in GG model

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

$$\sum_{i=1}^{N} \frac{1}{N} \, \delta_{\mathsf{X}_{i}(t)}$$

should converge to a process with density $u(\xi, \tau)$ solving

 $\partial_{\tau} u(\xi, \tau) = \partial_{\xi} (\operatorname{const} \sqrt{u(\xi, \tau)} \partial_{\xi} u(\xi, \tau))$

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Assume: for every E_1, E_2 we have $\Lambda(E_1, E_2) = \Lambda^*$ and $P(E_1, E_2, d\alpha) = P^*(d\alpha)$.

Theorem

If the stationary distribution $\pi_{\epsilon,N}$ of X(t) on $\mathcal{S}_{\epsilon,N}$ is reversible, then

$$\sigma(\mathcal{L}^*) \subset \left(-\infty, -\frac{1}{2}\Lambda^*\left[1-4\sigma_P^2\right]\sin^2\left[\frac{\pi}{N+2}\right]\right] \cup \{0\} \; ,$$

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where 0 is a simple eigenvalue corresponding to the constant eigenfunction.

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Spectral gap in the general case: Assumptions

Let $\pi_{\epsilon,N}$ be a reversible stationary distribution of \mathcal{L} on $\mathcal{S}_{\epsilon,N}$. Suppose that there exist a constant $\Lambda^* > 0$ and a probability measure P^* such that the following are satisfied:

- (i) Rate function Λ satisfies $\Lambda(E_1, E_2) \ge \Lambda^*$
- (ii) (Doeblin-type) There exists a constant $\beta > 0$ such that P satisfies the minorization condition $P(E_1, E_2, .) \ge \beta P^*(.)$
- (iii) The unique stationary distribution $\pi_{\epsilon,N}^*$ of \mathcal{L}^* on $\mathcal{S}_{\epsilon,N}$ (corresponding to Λ^* and P^*) is reversible.
- (iv) The measures $\pi_{\epsilon,N}$ and $\pi_{\epsilon,N}^*$ are uniformly equivalent, i.e. there exist two constants $0 < C_{\epsilon,N}^- \leq C_{\epsilon,N}^+ < \infty$ such that their Radon-Nikodym derivative satisfies $C_{\epsilon,N}^- \leq \frac{\pi_{\epsilon,N}(dx)}{\pi_{\epsilon,N}^*(dx)} \leq C_{\epsilon,N}^+$.

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Spectral gap for ${\cal L}$

Theorem

Then the spectrum of \mathcal{L} in $L^2_{\pi_{\epsilon,N}}$ satisfies

$$\sigma(\mathcal{L}) \subset \left(-\infty, -\beta \frac{C_{\epsilon,N}^-}{C_{\epsilon,N}^+} \Lambda^* \frac{1}{2} \left[1 - 4 \sigma_{P^*}^2\right] \sin^2 \left[\frac{\pi}{N+2}\right] \right] \cup \{0\} ,$$

where 0 is a simple eigenvalue.

Michiko SASADA, '11 (work in progress):

- $\frac{C}{M^2}$ spectral gap for stick models
- hope to extend methods to our energy exchange model

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Description of reversible product measures

Lemma (Reversible product measures and system size)

Let ν be a probability measure on \mathbb{R}_+ . Then the product (probability) measure $\mu(dx) = \nu(dx_1) \cdots \nu(dx_N)$ on \mathbb{R}_+^N is reversible for X(t) (with generator) for some N if and only if it is reversible for N = 2.

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Ра	rticular case)					

Assume that the rate function Λ and the transition kernel P are of the form

$$\Lambda(x_i, x_{i+1}) = \Lambda_{tot}(x_i + x_{i+1}) \Lambda_{part}\left(\frac{x_i}{x_i + x_{i+1}}\right)$$
$$P(x_i, x_{i+1}, d\alpha) = P\left(\frac{x_i}{x_i + x_{i+1}}, d\alpha\right) = P\left(\beta, d\alpha\right)$$

where

$$\beta = \frac{x_i}{x_i + x_{i+1}}$$

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As seen, they are satisfied in the GG model!

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Characterization of rev. product meas., $N \ge 2$

Theorem (Reversible product measures)

Suppose: Markov chain on [0,1] with kernel $P(\beta, d\alpha)$ (the energy exchange!) has a unique invariant distribution p(.). Suppose also that $\forall s > 0$ $\Lambda_{tot}(s) > 0$ and $\forall 0 < \beta < 1$ $\Lambda_{part}(\beta) > 0$. Then the product measure $\mu(dx) = \nu(dx_1) \cdots \nu(dx_N)$ is reversible for X(t) if and only if either of the following two holds:

- **(**degenerate) There exists $\epsilon > 0$ such that $\nu(dx_1) = \delta(\epsilon, dx_1)$.
- 2 (gamma) There exists $\epsilon > 0$ and d > 0 such that

$$\nu(dx_1) = \frac{dx_1}{\epsilon} \left[\frac{x_1}{\epsilon}\right]^{\frac{d}{2}-1} \frac{e^{-\frac{x_1}{\epsilon}}}{\Gamma(\frac{d}{2})}$$
$$p(d\beta) = d\beta \left[\beta \left(1-\beta\right)\right]^{\frac{d}{2}-1} \frac{\Gamma(d)}{\Gamma(\frac{d}{2})^2} \Lambda_{part} \frac{1}{Z}$$

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GG model, d = 3 revisited

In previous theorem Z is the normalizing constant, and

$$\int p(d\beta) \int P(\beta, d\alpha) \psi(\alpha, \beta) = \int p(d\beta) \int P(\beta, d\alpha) \psi(\beta, \alpha)$$

for all bounded $\psi : [0,1]^2 \to \mathbb{R}$.

GG-model, d = 3

$$\nu(dx_1) = \frac{dx_1}{\epsilon} \sqrt{\frac{x_1}{\epsilon}} \frac{2 e^{-\frac{x_1}{\epsilon}}}{\sqrt{\pi}}$$
$$\nu_{tot}(ds) = \frac{ds}{\epsilon} \left[\frac{s}{\epsilon}\right]^2 \frac{e^{-\frac{s}{\epsilon}}}{2} , \qquad \nu_{part}(d\beta) = d\beta \sqrt{\beta (1-\beta)} \frac{8}{\pi}$$
$$p(d\alpha) = d\alpha \sqrt{\alpha (1-\alpha)} \frac{8}{\pi} \Lambda_{part}(\alpha) \frac{1}{Z}$$

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Main result for GG, d = 3

Corollary

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

- The product measure $\mu(dx) = \nu(dx_1) \cdots \nu(dx_N)$ with $\nu(dx_1) = \frac{dx_1}{\epsilon} \sqrt{\frac{x_1}{\epsilon}} \frac{2e^{-\frac{x_1}{\epsilon}}}{\sqrt{\pi}}$ is the unique reversible product measure for X(t).
- **2** On every $S_{\epsilon,N}$ there exists a unique stationary distribution $\pi_{\epsilon,N}$. This measure is obtained by conditioning $\mu(dx)$.
- **3** The spectrum $\sigma(\mathcal{L})$ of the generator \mathcal{L} acting on $L^2_{\pi_{\epsilon,N}}$ satisfies

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

for some constant C, which may depend on the choice of Λ_{tot} .

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Main parts of proof

Comparison

2 Gap bound for simple model



Comparison method 1

Then the associated Dirichlet form

$$\mathcal{D}_{\epsilon,N}(A) = \int \pi_{\epsilon,N}(dx) A(x) [-\mathcal{L}A](x)$$

is defined for all $A \in L^2_{\pi_{\epsilon,N}}$, and has the representation

$$= \frac{1}{2} \sum_{i=1}^{N-1} \int \pi_{\epsilon,N}(dx) \Lambda(x_i, x_{i+1}) \int P(x_i, x_{i+1}, d\alpha) \left[A(T_{i,\alpha}x) - A(x) \right]^2.$$

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Comparison method 2

The basic idea to prove convergence rates for X(t) is to compare the spectral gap of its generator \mathcal{L} to that of a simple reference process. In order to distinguish these two generators we use a superscript \star

$$\mathcal{L}^{\star}A(x) = \Lambda^{\star} \sum_{i=1}^{N-1} \int P^{\star}(d\alpha) \left[A(T_{i,\alpha}x) - A(x) \right]$$
$$\mathcal{D}^{\star}_{\epsilon,N}(A) = \frac{1}{2} \int \pi^{\star}_{\epsilon,N}(dx) \sum_{i=1}^{N-1} \Lambda^{\star} \int P^{\star}(d\alpha) \left[A(T_{i,\alpha}x) - A(x) \right]^{2}$$

to denote the invariant measure, the generator and the corresponding Dirichlet form of the reference process.

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Spectral gap in the general case: Assumptions

Let $\pi_{\epsilon,N}$ be a reversible stationary distribution of \mathcal{L} on $\mathcal{S}_{\epsilon,N}$. Suppose that there exist a constant $\Lambda^* > 0$ and a probability measure P^* such that the following are satisfied:

- (i) Rate function Λ satisfies $\Lambda(E_1, E_2) \ge \Lambda^*$
- (ii) (Doeblin-type) There exists a constant $\beta > 0$ such that P satisfies the minorization condition $P(E_1, E_2, .) \ge \beta P^*(.)$
- (iii) The unique stationary distribution $\pi_{\epsilon,N}^*$ of \mathcal{L}^* on $\mathcal{S}_{\epsilon,N}$ (corresponding to Λ^* and P^*) is reversible.
- (iv) The measures $\pi_{\epsilon,N}$ and $\pi_{\epsilon,N}^{\star}$ are uniformly equivalent, i.e. there exist two constants $0 < C_{\epsilon,N}^{-} \leq C_{\epsilon,N}^{+} < \infty$ such that their Radon-Nikodym derivative satisfies $C_{\epsilon,N}^{-} \leq \frac{\pi_{\epsilon,N}(dx)}{\pi_{\epsilon,N}^{\star}(dx)} \leq C_{\epsilon,N}^{+}$.



Comparison method 3

Since we assume reversibility, the generator is self-adjoint, and hence we have the following variational characterization

$$\gamma = \inf \left\{ \frac{\mathcal{D}_{\epsilon,N}(A)}{\operatorname{Var}_{\epsilon,N}(A)} : A \in L^2_{\pi_{\epsilon,N}}, \operatorname{Var}_{\epsilon,N}(A) \neq 0 \right\}$$

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of the spectral gap γ of \mathcal{L} acting on $L^2_{\pi_{\epsilon,N}}$, where $\operatorname{Var}_{\epsilon,N}(A)$ denotes the variance of A with respect to $\pi_{\epsilon,N}$.

 $\mathcal{D}_{\epsilon,N}(A)$ can be bounded from below by using (i)-(iv), and $\operatorname{Var}_{\epsilon,N}(A)$ from above by using (iv).

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Hydrodynamical limit: simple cases

 If Λ ≡ const. and P(β, dα) = P(dα) (in fact, P(dα) need not be abs. cont.) then the limiting equation is

 $\partial_t u = C \Delta u;$

2 If $\Lambda(E_1, E_2) = E_1 + E_2$ and $P(\alpha) = \delta_{1/2}$, then the limiting equation is

 $\partial_{\tau} u(\xi,\tau) = \partial_{\xi} (C u(\xi,\tau) \partial_{\xi} u(\xi,\tau)) = C/2 \Delta u^{2}(\xi,\tau)$

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Summary

- Introduced a mesoscopic stochastic model close to GG model
- Formulated conditions ensuring appropriate lower bound $(\frac{1}{N^2})$ for spectral gap in terms of N
- Now one can attack hydrodynamic limit (à la Varadhan).
 BUT: it is a non-gradient system! (except for toy models)
- Tasks:
 - Prove hydrodynamic limit
 - Improve conditions, in particular, on bdedness away from 0 of Λ (numerical evidence!)
 - Return to Sz.-Tóth-approach



Vaserstein-distance

Recall that the definition of the Vaserstein-p distance is

$$\rho_p(\mu,\nu) = \inf_{\substack{X \sim \mu \\ Y \sim \nu}} [\mathbb{E}D(X,Y)^p]^{\frac{1}{p}} \quad \text{and set} \quad \rho(\mu,\nu) \equiv \rho_1(\mu,\nu)$$

where μ and ν are two probability measures on a compact metric space (S,d).

We will be using p = 2.

Furthermore, for p = 1 the duality

$$\rho(\mu,\nu) = \inf_{\substack{X \sim \mu \\ Y \sim \nu}} \mathbb{E}d(X,Y) = \sup_{f: \text{Lip}(f) \le 1} (\mu(f) - \nu(f))$$

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follows by the Kantorovich-Rubinstein theorem.

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Proof of convergence in Vaserstein-2 distance cont'd

Proposition (Rate of convergence in Vaserstein-2 distance)

Let U(t) and U'(t) be any two Markov chains generated by $\hat{\mathcal{L}}$ on $S_{\epsilon,N}$. Then

$$\rho_2(\mathsf{U}(t),\mathsf{U}'(t)) \le \rho_2(\mathsf{U}(0),\mathsf{U}'(0)) \exp\left(-\frac{1}{2}\left[1-4\,\sigma_P^2\right]\,\sin^2\left[\frac{\pi}{N+2}\right]t\right)$$
$$\le \epsilon\,N\,\sqrt{N-1}\,\exp\left(-\frac{1}{2}\left[1-4\,\sigma_P^2\right]\,\sin^2\left[\frac{\pi}{N+2}\right]t\right)$$

holds for all t.

- If $\sigma_P^2 < \frac{1}{4}$, then there exists a unique stationary distribution $\pi_{\epsilon,N}$ on each $S_{\epsilon,N}$.
- This rate of convergence is again $O(N^{-2})$, and thus optimal.

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