

LSI for Kawasaki dynamics with superquadratic single-site potential

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joint work with Felix Otto

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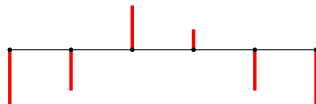
MAX-PLANCK-GESELLSCHAFT



Spin system

State space

Euclidean space \mathbb{R}^N



Hamiltonian

Function $H : \mathbb{R}^N \rightarrow \mathbb{R}$

H specified later

Gibbs measure

$\mu(dx) := Z^{-1} \exp(-H(x)) dx$

Kawasaki dynamics

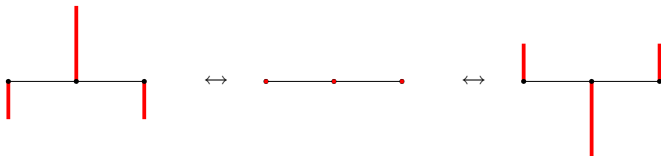
Stochastic process

$$dX_t = -A\nabla H(X_t)dt + \sqrt{2A}dB_t, \quad X_t \in \mathbb{R}^N$$

A second order difference operator
f.e. for the 1-d periodic lattice

$$A := N^2 \begin{pmatrix} 2 & -1 & 0 & 0 & \dots & -1 \\ -1 & 2 & -1 & 0 & \dots & 0 \\ 0 & -1 & 2 & -1 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & -1 & 2 & -1 & 0 \\ 0 & \dots & 0 & -1 & 2 & -1 \\ -1 & \dots & 0 & 0 & -1 & 2 \end{pmatrix}$$

Spin exchange between nearest neighbors



Kawasaki dynamics: simulation

System size

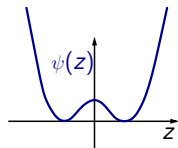
$$N = 6$$

Single-site potential

$$\psi(z) = (z^2 - 1)^2$$

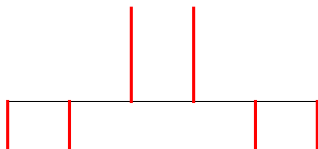
Hamiltonian

$$H(x) = \sum_{i=1}^6 \psi(x_i)$$



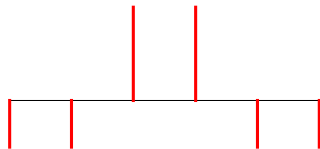
Deterministic gradient flow

$$dX_t = -A \nabla H(X_t) dt$$



Stochastic perturbation

$$+ \sqrt{2A} dB_t$$



Kawasaki dynamics

Questions

Is there an equilibrium state for X_t ?

If yes, does X_t approach the equilibrium?

In which sense and how fast?

Kawasaki dynamics

Questions

Is there an equilibrium state for X_t ?
If yes, does X_t approach the equilibrium?
In which sense and how fast?

Conservation of mean spin

$$\frac{1}{N} \sum_{i=1}^N x_i(t) = \frac{1}{N} \sum_{i=1}^N x_i(t=0) = m$$

New state space

$$\mathbb{R}^N \rightsquigarrow X_{N,m} = \left\{ x \in \mathbb{R}^N \mid \frac{1}{N} \sum_{i=1}^N x_i = m \right\}$$

Canonical ensemble

$$\mu \rightsquigarrow \mu = Z^{-1} \exp(-H(x)) \mathcal{H}_{\left\{ \frac{1}{N} \sum_{i=1}^N x_i = m \right\}}(dx)$$

μ is stationary for X_t .

Logarithmic Sobolev inequality

Definition $\mu(dx)$ satisfies LSI(ρ), if for all $f(x) \geq 0$

$$\text{Ent}(f\mu|\mu) := \int f \log f d\mu - \left(\int f d\mu \right) \log \left(\int f d\mu \right) \leq \rho^{-1} \int \frac{|\nabla f|^2}{2f} d\mu.$$

Observation 1 $|\nabla f|^2 \leq N^{-2} |\sqrt{A} \nabla f|^2.$

Observation 2 Let X_t be distributed as $f_t\mu$, then

$$\frac{d}{dt} \text{Ent}(f_t\mu|\mu) = - \int \frac{|\sqrt{A} \nabla f_t|^2}{2f_t} d\mu.$$

Consequence

If μ satisfies LSI(ρ), then $\text{Ent}(f_t\mu|\mu) \leq \exp(-N^{-2}\rho t) \text{Ent}(f_0\mu|\mu).$

Remark LSI is well adapted to the hydrodynamic limit $N \rightarrow \infty.$

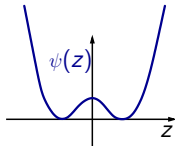
LSI for Kawasaki: known results

Quadratic case

Proposition (Landim, Panizo & Yau '02)

Assume

$$H(x) = \sum_{i=1}^N \psi(x_i), \quad \text{non-interacting}$$



$$\psi(z) = \frac{1}{2}z^2 + V_b(z), \quad z \in \mathbb{R} \quad \text{with} \quad |V_b|_\infty, |V_b'|_\infty, |V_b''|_\infty < \infty.$$

Then μ satisfies $\text{LSI}(\varrho)$.

The constant $\varrho > 0$ is **independent** of the system size N and the mean spin m .

Two different proofs

Landim, Panizo & Yau '02, Chafaï '03: Lu-Yau martingal method

Grunewald, Otto, Villani & Westdickenberg '09: Two-scale approach

LSI for Kawasaki: known results

Subquadratic case counterexample of Barthe & Wolff '09

$$\psi(z) = \begin{cases} z, & \text{for } z > 0 \\ \infty, & \text{else} \end{cases} \implies \begin{aligned} \text{SG}(\varrho) &\approx \frac{1}{m^2} \\ \text{LSI}(\varrho) &\approx \frac{1}{Nm^2} \end{aligned}$$

Superquadratic case Question raised by Varadhan '93

$$\begin{aligned} \psi(z) &= V_c(z) + V_b(z) \\ V_c''(z) &\geq c > 0 \quad \text{and} \quad |V_b|_\infty, |V_b'|_\infty < \infty. \end{aligned}$$

Conjecture by Landim, Panizo & Yau '02

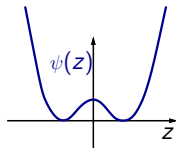
Partial answer for spectral gap by Caputo '02

LSI for Kawasaki: superquadratic case

Proposition (M. & Otto '10).

Assume

$$H(x) = \sum_{i=1}^N \psi(x_i), \quad \text{non-interacting}$$



with ψ is perturbed strictly convex i.e

$$\psi(z) = V_c(z) + V_b(z), \quad z \in \mathbb{R}$$

$$V_c''(z) \geq c > 0 \quad \text{and} \quad |V_b|_\infty, |V_b'|_\infty < \infty.$$

Then μ satisfies LSI(ρ), independent of N and m .

Remarks

Improves result of Caputo for spectral gap.

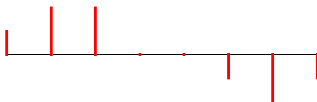
Two-scale approach

Coarse graining

N = size of the system

K = size of a block

M = number of blocks



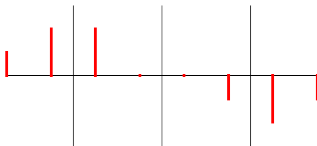
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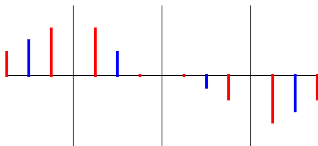
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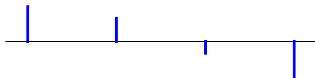
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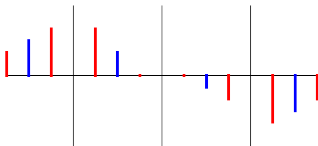
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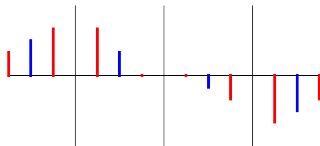
Two-scale approach

Coarse graining

N = size of the system

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M = number of blocks



Coarse graining operator

$$P\mathbf{x} := (y_1, \dots, y_M)$$

$$:= \left(\frac{1}{K} \sum_{i=1}^K x_i, \dots, \frac{1}{K} \sum_{i=N-K+1}^N x_i \right)$$

Decomposition of μ

$$\mu(d\mathbf{x}) = \mu(d\mathbf{x} | P\mathbf{x} = \mathbf{y}) \bar{\mu}(d\mathbf{y})$$

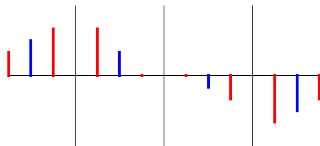
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Proposition (Two-scale criterion for LSI, GOVW '09)

Assume that

- $\kappa := \sup \left\{ \frac{\langle x, \text{Hess } H y \rangle}{|x| |y|} ; x \in \text{Ker } P, y \in (\text{Ker } P)^\perp \right\} < \infty,$
- $\mu(d\mathbf{x} | P\mathbf{x} = \mathbf{y})$ satisfies $\text{LSI}(\varrho_1)$ independent of N , m , and \mathbf{y} , (Mikro LSI)
- $\bar{\mu}(d\mathbf{y})$ satisfies $\text{LSI}(\varrho_1)$ independent of N and m . (Makro LSI)

Then μ satisfies the $\text{LSI}(\varrho)$, independent of N and m .

Adapted two-scale approach

Problem $\kappa \stackrel{!}{=} \infty$ for general $\psi = V_c + V_b$

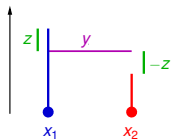
Adapted two-scale approach

Problem $\kappa \stackrel{!}{=} \infty$ for general $\psi = V_c + V_b$

Simplification Coarse graining of pairs i.e. $K = 2$

$$\mu(dx | P_X = y) = \bigotimes_{i=1}^M \mu \left(dx_{2i-1}, dx_{2i} \mid \frac{x_{2i-1} + x_{2i}}{2} = y_i \right)$$

Fluctuations of a spin pair



$$\mu \left(dx_1, dx_2 \mid \frac{x_1 + x_2}{2} = y \right) \approx \underbrace{\frac{\exp(-\psi(z+y) - \psi(-z+y))}{Z}}_{=: \nu(dz|y)} dz$$

$\nu(dz|y)$ is an one-dimensional measure

Crucial estimate for two-scale criterion

Lemma (Covariance estimate GOVW '09)

Assume that $\psi = V_c + V_b$. Then for $\int f(z)\nu(dz|y) = 1$

$$\text{cov}_{\nu(dz|y)}(g(z), f(z)) \leq C \sup_z |g'(z)| \left(\int \frac{|f'(z)|^2}{2f(z)} \nu(dz|y) \right)^{\frac{1}{2}}.$$

For the two-scale criterion: $g(z) = V_c'(-z + y) + V_c'(z + y)$

Case $V_c(z) = z^2$: $g'(z) = 4 \Rightarrow \kappa = \sup_z |g'(z)| < \infty$

Case $V_c(z) = z^4$: $g'(z) = 48zy \Rightarrow \kappa = \sup_z |g'(z)| = \infty$

Consequence

Improve the covariance estimate!

Hope

Convexity is "good".

Use the additional convexity of $z^4 \longleftrightarrow z^2$!

Crucial estimate: superquadratic case

Proposition (Brascamp & Lieb '76).

Assume $\mu(dz) = Z^{-1} \exp(-H(z))dz$, $z \in \mathbb{R}$ and $H''(z) > 0$.

Then $\text{var}_\mu(f) \leq \int \frac{|f'(z)|^2}{H''(z)} \mu(dz)$.

Proposition (Assymmetric Brascamp & Lieb, M. & Otto '10).

Assume $\mu(dz) = Z^{-1} \exp(-H(z))dz$, $z \in \mathbb{R}$ and $H''(z) > 0$.

Then $\text{cov}_\mu(g, f) \leq \sup_z \left| \frac{g'(z)}{H''(z)} \right| \int |f'(z)| \mu(dz)$.

Elementary proof using calculus.

Multidimensional version by Carlen, Cordero-Erausquin & Lieb '11.

Crucial estimate: superquadratic case

Corollary (Improved covariance estimate).

Assume that $\psi = V_c + V_b$. Then for $\int f(z)\nu(dz|y) = 1$

$$\begin{aligned} & \text{cov}_{\nu(dz|y)}(g, f) \\ & \leq C \sup_z \left| \frac{g'(z)}{V_c''(-z+y) + V_c''(z+y)} \right| \left(\int \frac{|f'(z)|^2}{f(z)} \nu(dz|y) \right)^{\frac{1}{2}}. \end{aligned}$$

Apply covariance estimate to $g(z) = V_c'(-z+y) + V_c'(z+y)$

$$\sup_z \left| \frac{g'(z)}{V_c'''(-z+y) + V_c'''(z+y)} \right| = \sup_z \left| \frac{V_c'''(-z+y) - V_c'''(z+y)}{V_c'''(-z+y) + V_c'''(z+y)} \right| \leq 2$$

Crucial estimate: superquadratic case

Corollary (Improved covariance estimate).

Assume that $\psi = V_c + V_b$. Then for $\int f(z)\nu(dz|y) = 1$

$$\begin{aligned} & \text{cov}_{\nu(dz|y)}(g, f) \\ & \leq C \sup_z \left| \frac{g'(z)}{V_c''(-z+y) + V_c''(z+y)} \right| \left(\int \frac{|f'(z)|^2}{f(z)} \nu(dz|y) \right)^{\frac{1}{2}}. \end{aligned}$$

Apply covariance estimate to $g(z) = V_c'(-z+y) + V_c'(z+y)$

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Two-scale criterion for LSI is satisfied for coarse-graining of pairs!

Open question

Hamiltonian with interaction

Proposition (M '09).

Assume

$$H(x) = \sum_{i=1}^N (x_i^2 + V_b(x_i)) + \varepsilon \sum_{i \sim j} x_i x_j, \quad \text{interacting}$$

$$|V_b|_\infty, |V_b'|_\infty, |V_b''|_\infty < \infty.$$

If $\varepsilon > 0$ is small enough, then μ satisfies $\text{LSI}(\varrho)$.

In this case $\varrho > 0$ is **independent** of the system size N and the mean spin m .

Generalize last statement to

$$H(x) = \sum_{i=1}^N (V_c(x_i) + V_b(x_i)) + \varepsilon \sum_{i \sim j} x_i x_j$$

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Generalize last statement to

$$H(x) = \sum_{i=1}^N (V_c(x_i) + V_b(x_i)) + \varepsilon \sum_{i \sim j} x_i x_j$$

Thank you for your attention.

Iterated of coarse graining of pairs

Coarse grained system $\bar{\mu}(dy) = Z^{-1} \exp(-\bar{H}(y)) \mathcal{H}(dy)$

Coarse grained Hamiltonian $\bar{H}(y) = \sum_{i=1}^{\frac{N}{2}} \mathcal{R}\psi(y_i)$

Renormalization operator $\mathcal{R} : \mathbb{R} \rightarrow \mathbb{R}$

$$\mathcal{R}\psi(z) = -\log \int \exp(-\psi(x_1) - \psi(x_2)) \mathcal{H}_{\lfloor \frac{x_1+x_2}{2} = z \rfloor}(dx_1, dx_2)$$

Lemma (Invariance under renormalization)

If ψ is perturbed strictly convex then $\mathcal{R}\psi$ also is perturbed strictly convex.

Lemma (Convexification of ψ by iterated renormalization)

There is K such that $\mathcal{R}^K \psi$ is uniformly strictly convex.

Macroscopic LSI by iterated coarse-graining and Bakry & Émery

Hierarchical criterion for LSI

Decomposition of μ $\mu(dx) = \int \mu(dx|Px = y) \bar{\mu}(dy)$

Decomposition of entropy $\bar{f}(y) := \int f(x)\mu(dx|Px = y)$, then

$$\text{Ent}(f\mu, \mu) = \int \text{Ent}(f\mu(dx|y), \mu(dx|y)) d\bar{\mu} + \text{Ent}(\bar{f}\bar{\mu}, \bar{\mu})$$

Microscopic scale ψ perturbed strictly convex
 $\Rightarrow \mu(dx|Px = y)$ satisfies LSI($\tilde{\varrho}$) i.e.

$$\int \text{Ent}(f\mu(dx|y), \mu(dx|y)) \bar{\mu}(dy) \leq \frac{1}{\tilde{\varrho}} \int \frac{|\nabla f(x)|}{2f(x)} \underbrace{\mu(dx|Px = y)}_{=\mu(dx)} \bar{\mu}(dy).$$

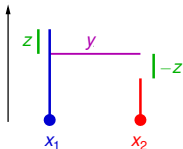
Macroscopic scale By assumption $\bar{\mu}$ satisfies LSI(ϱ_1) i.e.

$$\text{Ent}(\bar{f}\bar{\mu}, \bar{\mu}) \leq \frac{1}{\varrho_1} \int \frac{|\nabla \bar{f}(y)|}{2\bar{f}(y)} \bar{\mu}(dy).$$

Hierarchic criterion for LSI

Crucial estimate for hierachic criterion

$$\int \frac{|\nabla \bar{f}(y)|}{2\bar{f}(y)} \bar{\mu}(dy) \stackrel{!}{\leq} C \int \frac{|\nabla f(x)|}{2f(x)} \mu(dx)$$



Distribution of a pair

$$\mu(dx_1, dx_2 \mid \frac{x_1 + x_2}{2} = y) \approx \underbrace{\frac{\exp(-\psi(z+y) - \psi(-z+y))}{Z}}_{=: \nu(dz|y)} dz$$

Crucial estimate reduced to

Recall $\psi = V_c + V_b$. For all $f : \mathbb{R} \rightarrow \mathbb{R}$ with $\int f(z)\nu(dz|y) = 1$,

$$\text{cov}_{\nu(dz|y)} (V'_c(z+y) + V'_c(-z+y), f(z)) \stackrel{!}{\leq} C \left(\int \frac{|f'(z)|}{2f(z)} \nu(dz|y) \right)^{\frac{1}{2}}.$$

From quadratic to superquadratic potentials

Change the structure of the proof of GOVW '09

two-scale argument (big blocks) \rightsquigarrow iterative argument (block of pairs)

New tools to handle superquadratic potentials

generalized covariance estimate \rightsquigarrow Hierarchic criterion for LSI
 \rightsquigarrow Invariance of renormalization

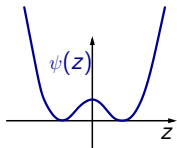
generalized local Cramér theorem \rightsquigarrow Convexification of $\mathcal{R}^K \psi$

Result for spectral gap by Caputo

Proposition (Caputo '02).

Assume

$$H(x) = \sum_{i=1}^N \psi(x_i), \quad \text{non-interacting}$$



$$\psi(z) = V_c(z) + V_b(z), \quad z \in \mathbb{R} \quad \text{with} \quad |V_b|_\infty, |V_b'|_\infty, |V_b''|_\infty < \infty,$$

$$V_c''(z) \geq c > 0, \quad \frac{1}{C} \leq \liminf \frac{V_c''(z)}{|z|^n} \leq \limsup \frac{V_c''(z)}{|z|^n} \leq C, \quad C > 0, \quad n \in [0, \infty).$$

Then μ satisfies $\text{SG}(\varrho)$.

The constant $\varrho > 0$ is **independent** of the system size N and the mean spin m .

Remark

Conservation of mean spin \rightsquigarrow long-range interaction.

Question

Similar result for LSI?