Energy Diffusion in a System of An-harmonic Oscillators

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Chain of Anharmonic oscillators

$p_i, q_i \in \mathbb{R}$, $i \in \Lambda$, $|\Lambda| = N$ or $\Lambda = \mathbb{Z}$.

$$\mathcal{H} = \sum_i \left[\frac{p_i^2}{2} + V(q_i - q_{i-1}) + U(q_j) \right]$$
$$= \sum_i e_i$$

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$$\begin{aligned} dq_i &= p_i \, dt \\ dp_i &= -\partial_{q_i} \mathcal{H} \, dt \end{aligned}$$

$$dQ_\beta = \frac{e^{-\beta \mathcal{H}}}{Z_\beta} dp dq \qquad \beta = T^{-1} > 0$$

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$$\jmath_{i,i+1} = -p_i V'(q_{i+1} - q_i) \qquad \text{hamiltonian energy currents}$$

Non-stationary behavior

We would like to prove that

$$\frac{1}{N}\sum_i G(i/N)e_i(N^2t) \underset{N\to\infty}{\longrightarrow} \int G(y)u(t,y)dy$$

with $u(t,y)$ solution of the nonlinear heat equation:

$$\partial_t u = \partial_y \mathcal{D}(u)\partial_y u$$

with the thermal conductivity defined by the *Green-Kubo formula*:

$$\mathcal{D}(u) = \chi_\beta^{-1}\sum_{i\in\mathbb{Z}}\int_0^\infty \left\langle \mathrm{J}_{i,i+1}(t)\mathrm{J}_{0,1}(0)\right\rangle_\beta \, dt \ , \qquad \beta = \beta(u)$$

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Not clear under which initial conditions such limit would be true

Equilibrium Fluctuations: Linear response

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Consider the system in equilibrium at temperature $T = \beta^{-1}$, and perturbe it at time 0 in atom 0 by adding some energy there: so we start with the measure

$$dQ'_\beta = \frac{e_0}{< e_0 >_\beta} dQ_\beta$$

We want to study the time evolution of

$$< e_i(t) >_{Q'_\beta} = \int e_i dQ'_{\beta,t} = \frac{< e_i(t) e_0(0) >}{< e_0 >}$$

Linear response

Assuming that the corresponding limits exist, we have that

$$\boxed{\mathcal{D} = \frac{\kappa}{\beta^2 \chi(\beta)} = \frac{< e_0 >_\beta}{\chi(\beta)} \lim_{t \to \infty} \frac{1}{t} \sum_{i \in \mathbb{Z}} i^2 < e_i(t) >_{Q'_\beta}}$$

with $\chi(\beta) = \sum_i (< e_i e_0 >_\beta - < e_i >_\beta < e_0 >_\beta)$.

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with $\chi(\beta) = \sum_i (< e_i e_0 >_\beta - < e_i >_\beta < e_0 >_\beta)$.
In fact, using stationarity and translation invariance

$$< e_0 >_\beta \sum_{i\in\mathbb{Z}} i^2 < e_i(t) >_{Q'_\beta} = \sum_{i\in\mathbb{Z}} i^2 < (e_i(t) - e_i(0)) e_i(0) >_\beta$$

$$= 2 \int_0^t ds \int_0^s d\tau \sum_i \left\langle j_{i,i+1}(s-\tau) j_{0,1}(0) \right\rangle$$

$$\xrightarrow[t\to\infty]{} 2 \int_0^\infty \sum_i \left\langle j_{i,i+1}(s) j_{0,1}(0) \right\rangle \, ds$$

Linearized heat equation

Define

$$C(i,j,t) =< e_i(t) e_j(0) >_\beta \; - \; \bar{e}^2$$

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Conjecture:

$$\boxed{NC([Nx],[Ny],N^2 t) \underset{N\to\infty}{\longrightarrow} (2\pi\mathcal{D})^{-1/2} \exp\left(-\frac{(x-y)^2}{2t\mathcal{D}}\right)}$$

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this is more challenging than proving existence for $\mathcal{D}$.

How to prove this?

Define, for a *good* choice of a sequence of smooth local functions $\mathcal{F}_n$

$$\Phi_n = j_{0,1} - \mathcal{D}(e_1 - e_0) - L\mathcal{F}_n$$

with L the generator of the dynamics,

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and pick a nice test function $G(x)$:

$$\frac{1}{N}\sum_{i,j} G\left(\frac{i}{N}\right) F\left(\frac{j}{N}\right)\left[C(i,j,N^2t) - C(i,j,0)\right]$$

$$= \frac{1}{N}\sum_{i,j} G\left(\frac{i}{N}\right) F\left(\frac{j}{N}\right)\left\langle (e_i(N^2t) - e_i(0))e_j(0)\right\rangle$$

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$$= \int_0^t \sum_{i,j} \nabla G\left(\frac{i}{N}\right) F\left(\frac{j}{N}\right)\left\langle j_{i,i+1}(N^2s)e_j(0)\right\rangle ds$$

$$= \int_0^t \frac{1}{N} \sum_{i,j} \Delta G\left(\frac{i}{N}\right) F\left(\frac{j}{N}\right) \mathcal{D} \left\langle e_i(N^2 s) e_j(0) \right\rangle ds$$

$$+ \int_0^t \frac{1}{N^2} \sum_{i,j} \nabla G\left(\frac{i}{N}\right) F\left(\frac{j}{N}\right) \left\langle (N^2 L) \tau_i \mathcal{F}_n(N^2 s) e_j(0) \right\rangle ds$$

$$+ \int_0^t \sum_{i,j} \nabla G\left(\frac{i}{N}\right) F\left(\frac{j}{N}\right) \left\langle \tau_i \Phi_n(N^2 s) e_j(0) \right\rangle ds$$

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$$\sim \int_0^t \frac{1}{N^2} \sum_{i,j} \Delta G\left(\frac{i}{N}\right) F\left(\frac{j}{N}\right) \mathcal{D} N C(i, j, N^2 t) ds$$

$$+ \frac{1}{N^2} \sum_{i,j} \nabla G\left(\frac{i}{N}\right) F\left(\frac{j}{N}\right) \left\langle \tau_i (\mathcal{F}_n(N^2 t) - \mathcal{F}_n(0)) e_j(0) \right\rangle ds$$

$$+ \int_0^t \sum_{i,j} F\left(\frac{j}{N}\right) \nabla G\left(\frac{i}{N}\right) \left\langle \frac{1}{2k} \sum_{|i-l| \le k} \tau_l \Phi_n(N^2 s) e_j(0) \right\rangle ds$$

$$\Phi_n = \jmath_{0,1} - \mathcal{D}(e_1 - e_0) - LF_n$$

$$\hat{\Phi}_{n,k} = \frac{1}{2k} \sum_{|j| \le k} \tau_j \Phi_n$$

By Schwarz we can bound the square of the last term by

$$\|F\|^2 \bar{e}^2 \left\langle \left(\int_0^t N \sum_i G'\left(\frac{i}{N}\right) \tau_i \hat{\Phi}_{n,k}(N^2 s) ds \right)^2 \right\rangle$$

$$= C \left\langle \left(\int_0^{N^2 t} \frac{1}{N} \sum_i G'\left(\frac{i}{N}\right) \tau_i \hat{\Phi}_{n,k}(s) ds \right)^2 \right\rangle$$

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For a deterministic hamiltonian infinite dynamics, I do not know how to show that this variance is small.

Stochastic dynamics perturbations

For stochastic dynamics there is a technique to prove this (in some cases...):

Varadhan's Non Gradient methods.

- S.R.S. Varadhan (1990): Non-gradient Ginzburg-Landau conservative model (*reversible*).

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- Romero (Dauphine-PhD thesis 2010): Energy conserving momentum dynamics (non-linear vector fields, *reversible*).

Varadhan's non-gradient method

For stochastic dynamics, roughly the idea is the following:

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How can the space-time variance be small?
For the finite set $\Lambda_k = \{-k, \dots, k\}$, consider the generator L_{Λ_k}, with free B.C. The corresponding dynamics conserve the energy of the box $\sum_{i \in \Lambda_K}$, if the *noise* is sufficiently nice (ellipticity, spectral gap ...), there will be ergodicity in the corresponding microcanonical surface, and it will be possible to solve the equation

$$L_{\Lambda_K} u_k = \frac{1}{2k} \sum_{i=-k}^{k-1} j_{i,i+1}$$

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going back to the full generator of the infinite dynamics:

$$\frac{1}{2K} \sum_{i=-k}^{k-1} \mathrm{J}_{i,i+1} = -(L - L_{\Lambda_k}) u_k + L u_k$$

It is the boundary term $(L - L_{\Lambda_k}) u_k$ that gives origin to the gradient $\mathcal{D}_T (e_k - e_{-k})$, in the proper limit.

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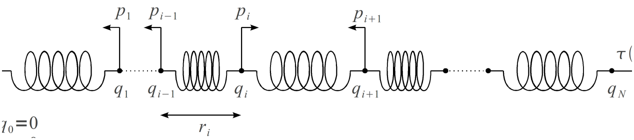
This requies some work and two ingredients: bounds on the spectral gap and a sector condition.

Chain un unpinned anharmonic oscillators with conservative noise

Joint work with *Makiko Sasada* (Keio University, Tokyo).
Take $U = 0$ (unpinned), and

$$r_i = q_i - q_{i-1}$$



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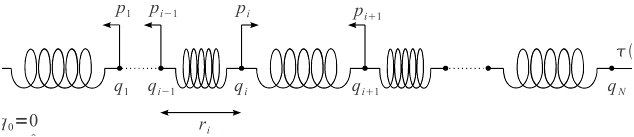

Equilibrium measure are product:

$$dQ_\beta = \prod_i \frac{e^{-\beta(p_i^2/2+V(r_i))}}{Z_\beta} dp_i dr_i \qquad \beta = T^{-1} > 0$$

$V \in \mathcal{C}^2$, $0 < C_- \le V''(r) \le C_+ < +\infty$.

Energy Conserving Noise

We use the vector fields tangent to the microcanonical surface:

$$Y_{i,j} = p_i \partial_{r_j} - V'(r_j)\partial_{p_i},$$
$$X_i = Y_{i,i}$$

The Hamiltonian vector field is

$$A = \sum_i (p_i - p_{i-1})\partial_{r_i} - V'(r_i)(\partial_{p_i} - \partial_{p_{i-1}}) = \sum_i (X_i - Y_{i-1,i})$$

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We add stochastic dynamics with generator defined by

$$S = \sum_i (X_i^2 + Y_{i,i+1}^2)$$

$$L = A + S$$

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It will be interesting extend this to different type of noise or chaotic mechanism.

Currents

$$
\begin{aligned}
\mathrm{J}^{a}_{i,i+1} &= Y_{i,i+1} e_i = -p_i V'(r_{i+1}) \\
\mathrm{J}^{s}_{i,i+1} &= Y^2_{i,i+1} e_i = -p_i^2 V''(r_{i+1}) + V'(r_{i+1})^2
\end{aligned}
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NON GRADIENT CURRENTS

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NON GRADIENT CURRENTS

In the *harmonic* case ($V(r) = r^2/2$) we have the decomposition:

$$\mathrm{j}_{0,1} = \mathcal{D}(e_1 - e_0) + LF$$

for a homogeneous second order polynome $F(r,p)$ and $\mathcal{D}$ constant.

$$\Phi_n = j_{0,1} - \mathcal{D}_T(e_1 - e_0) - LF_n$$
$$\hat{\Phi}_{n,K} = \frac{1}{2K}\sum_{|j|\le K}\tau_j\Phi_n$$

By a general inequality valid for all Markov processes:

$$\left\langle\left(\int_0^t N\sum_j G'(i/N)\tau_i\hat{\Phi}_{n,K}(N^2 s)ds\right)^2\right\rangle$$
$$\le Ct\left\langle\sum_i G'(i/N)\tau_i\hat{\Phi}_{n,K}, (-S)^{-1}\sum_i G'(i/N)\tau_i\hat{\Phi}_{n,K}\right\rangle$$
$$\sim\le Ct\|G'\|_{L^2}^2 K\left\langle\hat{\Phi}_{n,K}, (-S_{\Lambda_K})^{-1}\hat{\Phi}_{n,K}\right\rangle$$

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$$\sim\le Ct \|G'\|^2_{L^2} K \left\langle \hat{\Phi}_{n,K}, (-S_{\Lambda_K})^{-1} \hat{\Phi}_{n,K} \right\rangle$$

We are left to prove that this is negligeable as $N \to \infty$, $K \to \infty$ and $n \to \infty$.

Microcanonical variance

$< \cdot >_{K,E}$: microcanonical expectation on the energy shell

$$\Sigma_{K,E} = \left\{ (r_1, p_1, \dots, r_K, p_K) : \sum_{i=1}^{K} e_i = KE \right\}$$

Hypothesis on $V \implies$ connected surface.

Microcanonical variance

$< \cdot >_{K,E}$: microcanonical expectation on the energy shell

$$\Sigma_{K,E} = \left\{ (r_1, p_1, \dots, r_K, p_K) : \sum_{i=1}^{K} e_i = KE \right\}$$

Hypothesis on $V \Longrightarrow$ connected surface.
For two local functions f, g define

$$\langle\!\langle f, g \rangle\!\rangle = \lim_{K \to \infty} \frac{1}{K} \left\langle \sum_{i=-k+\ell}^{k-\ell} \tau_i f, (-S_K)^{-1} \sum_{i=-k+\ell}^{k-\ell} \tau_i g \right\rangle_{K,E}$$

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We need to prove that there exists F_n such that

$$\langle\langle \Phi_n, \Phi_n \rangle\rangle \longrightarrow 0$$

for $\Phi_n = j_{0,1} - \mathcal{D}(e_1 - e_0) - LF_n$.

variational formulas

Let $\Phi = X_0 F + Y_{0,1} G$, for some local F, G, then

$$\lim_{K\to\infty} \frac{1}{2k} \left\langle \sum_{i=-k+\ell}^{k-\ell} \tau_i \Phi, (-S_K)^{-1} \sum_{i=-k+\ell}^{k-\ell} \tau_i \Phi \right\rangle_{k,E} = \langle\!\langle \Phi_n, \Phi_n \rangle\!\rangle$$

$$\leq \sup_{(\xi^0,\xi^1)\text{closed}} \left\{ 2 < F, \xi^0 > +2 < G, \xi^1 > -\gamma \left(< (\xi^0)^2 + (\xi^1)^2 > \right) \right\}$$

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Def: $(\xi^0, \xi^1) \in L^2 \times L^2$ is a closed form if

$$X_i(\tau_j \xi^0) = X_j(\tau_i \xi_0) \qquad Y_{j,j+1}(\tau_i \xi^1) = Y_{i,i+1}(\tau_j \xi^1)$$

$$X_i(\tau_j \xi^i) = Y_{j,j+1}(\tau_i \xi^0) \qquad i \neq j, j+1$$

$$\ldots$$

exact forms

We need to show that closed form are approximated (in $L^2(Q_\beta)$) by exact forms:
Def: $(\xi^0, \xi^1) \in L^2 \times L^2$ is an exact form if there exists F local and a constant $a \in \mathbb{R}$ such that

$$\xi^0 = X_0(\sum_{i\in\mathbb{Z}} \tau_i F)$$

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This is proven by a careful construction, integrating the form

$$\{\xi_j^m, j = 1, \dots, K, m = 0, 1\}$$

on the microcanonical surface $\Sigma_{E,K}$, that has the same cohomology of the 2K-sphere, and controlling the boundary conditions as $K \to \infty$, with the spectral gap on S_K.

Ingredients to prove this:

- Spectral gap bound for S_K: $SG(S_K) \geq CK^{-2}$.
- *Sector condition*: $|< vAu >|^2 \leq C < v(-S)v >< u(-S)u >$.

- Spectral gap bound for S_K: $SG(S_K) \geq CK^{-2}$.

i.e. for any smooth local f such that $< f >_{K,E} = 0$

$$< f^2 >_{K,E} \leq \; C_1 \sum_{i=1}^{K} \left\langle (X_i f)^2 \right\rangle_{K,E} + C_2 K^2 \sum_{i=1}^{K-1} \left\langle (Y_{i,i+1} f)^2 \right\rangle_{K,E}$$

$$\begin{aligned} Y_{i,i+1} &= p_i \partial_{r_{i+1}} - V'(r_{i+1}) \partial_{p_i}, \\ X_i &= Y_{i,i} = p_i \partial_{r_i} - V'(r_i) \partial_{p_i}, \end{aligned}$$

Sector Condition

For any i decompose $f = f_{i,odd} + f_{i,even}$

$$f_{i,odd}(p) = \frac{1}{2}(f(p^{(i)}) - f(p)), \qquad f_{i,even}(p) = \frac{1}{2}(f(p^{(i)}) + f(p)),$$

with $p_i^{(i)} = -p_i$ and $p_j^{(i)} = p_j$ if $j \neq i$.

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$$\begin{aligned}
\langle vX_i u \rangle &= \left\langle v_{i,odd} X_i u_{i,even} \right\rangle + \left\langle v_{i,even} X_i u_{i,odd} \right\rangle \\
&= \left\langle v_{i,odd} X_i u_{i,even} \right\rangle - \left\langle u_{i,odd} X_i v_{i,even} \right\rangle \\
&\leq \left\langle v_{i,odd}^2 \right\rangle^{1/2} \left\langle (X_i u_{i,even})^2 \right\rangle^{1/2} + \left\langle u_{i,odd}^2 \right\rangle^{1/2} \left\langle (X_i v_{i,even})^2 \right\rangle^{1/2} \\
&\leq C \left\langle (X_i v)^2 \right\rangle^{1/2} \left\langle (X_i u)^2 \right\rangle^{1/2} + \left\langle (X_i u)^2 \right\rangle^{1/2} \left\langle (X_i v)^2 \right\rangle^{1/2}
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\end{aligned}$$

and similarly for $< vY_{i-1,i}u >$.

$$\Longrightarrow \quad |\langle vAu \rangle| \le C \langle v(-S)v \rangle \langle u(-S)u \rangle.$$

equilibrium fluctuations

Equivalently we can express the result in term of the fluctuation field

$$Y^N = \frac{1}{\sqrt{N}} \sum_i \delta_{i/N} \{e_i(0) - e\}$$

It converges in law to a delta correlated centered gaussian field Y

$$\mathbb{E}[Y(F)Y(G)] = \chi \int F(y)G(y)dy$$

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Theorem

$$Y_t^N = \frac{1}{\sqrt{N}} \sum_i \delta_{i/N} \left\{\epsilon_i(N^2 t) - e\right\}$$

converges in law to the solution of the linear SPDE

$$\partial_t Y = \mathcal{D}\, \partial_y^2 Y \; dt + \sqrt{2\mathcal{D}\chi}\; \partial_y B(y,t)$$

proof of spectral gap bound

start with the martingale decomposition:

$$\mathcal{G}_k = \sigma\left\{e_1, \dots, e_k, p_{k+1}, r_{k+1}, \dots, p_L, r_L\right\}$$

$$f_k := E[f|\mathcal{G}_k], \qquad f_L = f_L(e_1, \cdots, e_L)$$

$$< f^2 >_{L,E} = \sum_{k=0}^{L-1} < (f_k - f_{k+1})^2 >_{L,E} + < f_L^2 >_{L,E}$$

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each X_k^2 has his uniform spectral gap in the corresponding microcanonical surface ($X_k e_k = 0$):

$$< f^2 >_{L,E} \leq C \sum_{k=0}^{L-1} < (X_{k+1} f_k)^2 >_{L,E} + < f_L^2 >_{L,E}$$

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$$< (Y_{k,k+1} f_L)^2 >_{L,E} \sim \left\langle e_k e_{k+1} \left[(\partial_{e_k} - \partial_{e_{k+1}}) f_L \right]^2 \right\rangle_{L,E}$$

Dirichlet form of the Ginzburg Landau model!

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Dirichlet form of the Ginzburg Landau model! We are left to prove G for this GL model:

$$< f_L^2 >_{L,E} \leq C_2 L^2 \sum_{k=1}^{L-1} \left\langle e_k e_{k+1} \left[(\partial_{e_k} - \partial_{e_{k+1}}) f_L \right]^2 \right\rangle_{L,E}$$

proof of the spectral gap bound

The microcanonical marginal density on the energies $e_1, \dots, e_L$ has a linear behavior at large values, and not strictly convex, also the weight $e_k e_{k+1}$ does not allow easy telescoping arguments.

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The microcanonical marginal density on the energies $e_1, \dots, e_L$ has a linear behavior at large values, and not strictly convex, also the weight $e_k e_{k+1}$ does not allow easy telescoping arguments.
Caputo approach + a smart telescoping + the elementary inequality

$$\int_0^1 g(t)^2 dt \ \leq \ \frac{1}{2} \int_0^1 g'(t)^2 t(1-t) dt$$