Non-equilibrium statistical mechanics of non-linear, thermally driven, Hamiltonian systems

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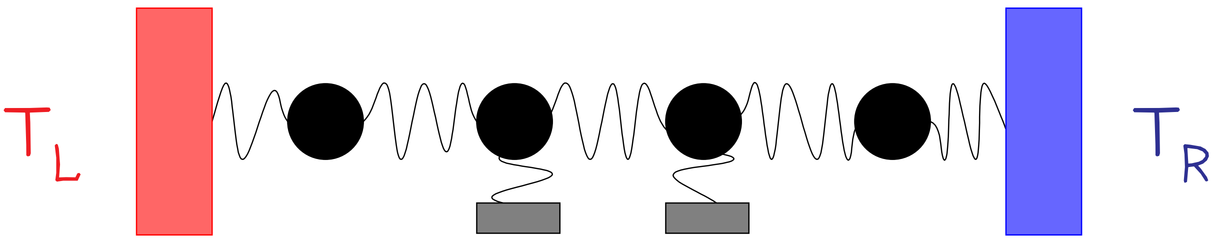
I. The models



The chain: - Finite
- Anharmonic
- Confining
- Transmits energy

$$H_C = \sum_{i=1}^{n} \frac{p_i^2}{2} + V(q)$$

$$V(q) = \sum_{1}^{n} V_1(q_i) + \sum_{1}^{n-1} V_2(q_i - q_{i+1})$$

quadratic at infinity (+lower order terms)

$(\nabla_{q_i} \nabla_{q_{i+1}} V)$ is a definite matrix , $\forall q$

NOT weak coupling

Martin Hairer:

Convex at infinity and
1-particle potential weaker than
inter-particle coupling

Favor transport of energy

Modeling of heat bath and its coupling to the chain
``Linear wave equation coupled linearly to the chain''

$$H = \frac{p^2}{2} + V(q) + \sum_k k^2 \frac{\varphi_k^2}{2} + \frac{\pi_k^2}{2}$$
$$+ q \sum \varphi_k \alpha_k$$

Equations of motion
(for <u>one</u> particle and one bath)

$$\dot{q} = p$$
$$\dot{p} = -V'(q) - \sum \varphi_k \alpha_k$$
$$\dot{\varphi}_k = \pi_k$$
$$\dot{\pi}_k = -k^2 \varphi_k - q \alpha_k$$

Since equ. for φ and π is linear, we can integrate. Let

$$\Phi = \begin{pmatrix} \varphi_k \\ \pi_k \end{pmatrix}, \; A = \begin{pmatrix} \alpha_k \\ 0 \end{pmatrix}, \; \mathcal{L} = \begin{pmatrix} 0 & 1 \\ -k^2 & 0 \end{pmatrix}$$

Then

$$\dot{\Phi}(t) = \mathcal{L}\Phi(t) - q(t)A$$

$$\Phi(t) = e^{\mathcal{L}t}\Phi(0) - \int_0^t ds\, q(s) e^{\mathcal{L}(t-s)} A$$

(Ford-Kac-Mazur) Substitute

$$\dot{q} = p$$

$$\dot{p} = -V'(q) - \sum_k \Phi_k(0) e^{-\mathcal{L}_k t} A_k$$

$$+ \sum_k \alpha_k^2 \int_0^t ds\, q(s) D_k(t-s)$$

$$\equiv -V'(q) + r$$

$$D_k(t-s) \approx \sin(k(t-s))/k$$

Assumptions about nature of coupling $q\sum \varphi_k \alpha_k$:

$$\alpha_k = \frac{ik\lambda}{(k^2+\gamma^2)^{1/2}}$$

Then we get from first term in r:

$$\sum \Phi_k(0)\cdot e^{-\mathcal{L}_k t} A_k$$

a variance

$$\sum_{k,k'} \langle \Phi_k(0)\cdot e^{-\mathcal{L}_k t} A_k \; \Phi_{k'}(0)\cdot e^{-\mathcal{L}_{k'} t} A_{k'} \rangle$$

$$\sim \int \frac{\lambda^2}{\beta(k^2+\gamma^2)} e^{ik(t-s)} dk$$

$$\sim \frac{\lambda^2}{\beta} e^{-\gamma|t-s|}$$

(Tropper) This is Markovian but noise is <u>not</u> white

We now introduce irreversibility by going to an ensemble average = temperature of the heat bath.

Assume the $\Phi_k \equiv \Phi_k(0)$ are random (Gaussian) with covariance

$$\langle \Phi_k \cdot A_k \; \Phi_{k'} \cdot A_{k'} \rangle = \frac{\delta_{kk'}}{\beta} \left(A_k \, , \begin{pmatrix} k^2 & 0 \\ 0 & 1 \end{pmatrix} A_{k'} \right)$$

Can also take (for example)

$$\alpha_k = \sum_m \frac{ik\lambda}{(k^2 + \gamma_m)^{1/2}}$$

(Jakšič-Pillet need less!
Not quite Markovian)

We get finally

$$dq = p\,dt$$
$$dp = -V'(q)\,dt + r\,dt$$
$$dr = -\gamma r\,dt + \lambda^2 q\gamma\,dt - \lambda\sqrt{\frac{2\gamma}{\beta}}\,d\omega$$

(ω is Wiener, r auxiliary variable)

Chain: Similar

$$dq_i = p_i\,dt \qquad i = 1,\ldots,n$$

$$dp_i = -\partial_{q_i} V\,dt \qquad i = 2,\ldots,n-1$$

$$dp_1 = -\partial_{q_1} V\,dt + r_1\,dt$$

$$dp_n = -\partial_{q_n} V\,dt + r_n\,dt$$

$$dr_1 = -\gamma_1 r_1\,dt + \lambda^2 q_1 \gamma_1\,dt - \sqrt{\frac{2\gamma_1}{\beta_L}}\lambda\,d\omega_1$$

$$dr_n = -\gamma_n r_n\,dt + \lambda^2 q_n \gamma_n\,dt - \sqrt{\frac{2\gamma_n}{\beta_R}}\lambda\,d\omega_n$$

Stochastic Differential Equation (SDE),
Markov Diffusion process,

only end of chain shaken,
"boundary driven"
no thermostats at other sites, not
weak coupling

II. Techniques and results

Remark: If $|\lambda| \geq \lambda_{crit}$, then system becomes unstable due to the retro-action $(\lambda^2 \ldots)$

Many authors absorb $-\lambda^2$ into "free" Hamiltonian
This is natural if model is supposed to describe dipole approximation.

We shall just assume $|\lambda| < \lambda_{crit}$. This is not a perturbative restriction!

THEOREM: The system SDE has a stationary state ρ with C^∞ density, also called ρ. For all values of the temperature difference and the coupling, this state is
unique,
mixing,
and "every" initial distribution converges to the stationary state

Mixing:

$$\lim_{t\to\infty} \langle F \cdot S^t G \rangle_\rho = \langle F \rangle_\rho \langle G \rangle_\rho$$

Invariant density ρ is solution of

$$L^T \rho = 0$$

where L is "Liouvillian"

Omitting all coefficients

$$L \approx \partial_{r_1}^2 - (r_1 - q_1)\partial_{r_1} + r_1 \partial_{p_1}$$
$$+ \partial_{r_n}^2 - (r_n - q_n)\partial_{r_n} + r_n \partial_{p_n}$$
$$+ \sum_i \left(p_i \partial_{q_i} - \partial_{q_i} V \partial_{p_i} \right)$$

A few ideas of proof:

1) Existence

Spectral properties of generator

$$dx(t) = b(x(t)) + \sigma\, d\omega(t)$$

Consider

$$E(f(x(t))|\mathcal{F}^s) = S^{t-s} f(x(s))$$

Study $K \equiv e^{-\beta_0 G/2} L e^{\beta_0 G/2}$ on space with weight dx (or L on space with $e^{-\beta_0 G/2}$), with $\beta_0 \sim 1/\text{mean temp.}$

$$G(p,q,r) = H_c(p,q) + \frac{r_1^2}{2\lambda^2} - q_1 r_1 + \frac{r_n^2}{2\lambda^2} - q_n r_n$$

N.B. If $\beta_L = \beta_R = \beta_0$ then $\rho = e^{-\beta_0 G}$ is density of invariant measure.

$$K \approx \partial_{r_1}^2 + (r_1 - q_1)^2 + r_1 \partial_{p_1}$$

$$+ 1 \leftrightarrow n + \sum_i \left(p_i \partial_{q_i} - \partial_{q_i} V \partial_{p_i} \right)$$

THEOREM: Uniform hypoellipticity bound: Let

$$\Lambda^2 = 1 + P^T P + Q^T Q + R^T R$$

where
$$P_j \sim p_j + \partial_{p_j}$$

$$Q_j \sim \partial_{q_j} V + \partial_{q_j} \sim q_j + \partial_{q_j}$$

$$R_1 \sim \lambda^{-2} r_1 - q_1 + \partial_{r_1}$$

$$R_n \sim \lambda^{-2} r_n - q_n + \partial_{r_n}$$

Then $\|Kf\| + \|f\| \geq C \|\Lambda^{4^{-n}} f\|, \quad C > 0$

COROLLARY: $\Lambda^2 \approx$ "Harmonic oscillator" (compact resolvent)

$\Rightarrow K$ has discrete spectrum

COROLLARY: Eigenvector of L^T with eigenvalue 0 exists and is density of invariant measure

Pf: Global version of ``Kolmogorov Equation'' (Hörmander). Example:

$$\partial_x^2 + x\partial_y \qquad \approx \exp\left(-\frac{x^2}{t} + \frac{3xy}{t^2} - \frac{3y^2}{t^3}\right)$$

In our case: noise coupling $\quad (\partial_y^2)^{1/2}$ Induction over sites of chain

Essentially

$$Q_j = [P_j, K]$$

$$P_j = -(\nabla_{q_j} \nabla_{q_{j-1}} V)^{-1} [Q_{j-1}, K]$$

coupling is effective

``Global'': $q \in \mathbb{R}^d$

New proof with M. Hairer

$$K = X_0 + \sum_{i=1}^{s} X_i^* X_i$$

$$X_0 \approx p\partial_q + V'\partial_p$$

$$X_i \approx a_i \partial$$

$$g_0 = G^{-3/2-\ell/m}$$

$$A_{-1} = \{X_1, \ldots, X_s\}$$

$$A_0 = \{g_0 X_0, X_1, \ldots, X_s\}$$

$$A_\ell = A_{\ell-1} \cup [g_0 X_0, A_{\ell-1}]$$

$$\Lambda^2 \equiv 1 + \sum_{A \in A_{2n+1}} A^* A$$

Usually:

$$\Lambda^2 = 1 - \sum_i \partial_{x_i}^2$$

$$\Lambda^2 = 1 - \sum_i \partial_{x_i}^2 + \sum_i x_i^2$$

$$\|Kf\| + \|f\| \geq \|\Lambda^{16^{-n}} f\| + \|G^{\varepsilon} f\|$$

$$X_1 = c_L \partial_{r_L} \,, \qquad X_3 = c_R \partial_{r_R}$$

$$X_2 = a_L(r_L - \lambda^2 q_1) \,, \qquad X_4 = a_R(r_R - \lambda^2 q_1)$$

$$X_0 = -r_L \partial_{p_1} + b_L(r_L - \lambda^2 q_1)\partial_{r_L}$$

$$-r_R \partial_{p_n} + b_R(r_R - \lambda^2 q_n)\partial_{r_R}$$

$$-p\partial_q - V'(q)\partial_p$$

2) Uniqueness "Control Theory"

THEOREM: The boundary noise can drive the system from any phase space point r,p,q to any other point r',p',q' in any given time $\tau > 0$.

This is generally improbable but never impossible.

Combining results of Stroock-Varadhan and Kunita, one shows that the support of ρ equals the set of reachable points (everything!). Thus, ρ is strictly positive and uniqueness follows.

III. Energy flux and entropy

Model is Hamiltonian setup

$$\begin{array}{ccccc} \text{Field theory} & \leftrightarrow & H_C & \leftrightarrow & \text{Field theory} \\ \downarrow & & \downarrow & & \downarrow \\ r_1 & \leftrightarrow & H_{eff} & \leftrightarrow & r_n \end{array}$$

$$\exp(-\beta H_{eff}(p,q)) \approx \int dr \exp(-\beta G(p,q,r))$$

Define energy flux by

$$\Phi \equiv \partial_t S^t H_{eff} = LH_{eff} = \Phi_L + \Phi_R$$

$$\approx (r_1 - q_1)p_1 + (r_n - q_n)p_n$$

By Hamiltonian nature: $\langle \Phi \rangle_\rho = 0$

so $\langle \Phi_L \rangle_\rho = -\langle \Phi_R \rangle_\rho$

Define (thermodynamic) entropy production rate by

$$\sigma \equiv \frac{\Phi_L}{T_L} + \frac{\Phi_R}{T_R}$$

THEOREM: The mean entropy production satisfies

$$\langle \sigma \rangle_\rho \leq 0$$

It is non-zero iff $T_L \neq T_R$

COROLLARY: The mean energy flow $\langle \Phi_L \rangle_\rho = -\langle \Phi_R \rangle_\rho$ is zero iff $T_L = T_R$.

Remark: Introduce "effective ρ" (independent of r if $T_L = T_R$: $e^{-\beta H_{eff}}$):

$$\hat{\rho} \equiv \rho \exp((r_1 - q_1)^2/2T_L + (r_n - q_n)^2/2T_R)$$

One shows $\langle \sigma \rangle_\rho \leq 0$ by identifying it with something like

$$\langle \sigma \rangle_\rho \approx -\langle |\nabla_r \log \hat{\rho}|^2 \rangle_\rho$$

One then shows that the square cannot vanish if $T_L \neq T_R$ using $L^T \rho = 0$.

Relation with Gibbs entropy

Given any initial density f_0, define f_t by $f_t = \exp(tL^T)f_0$

Set

$$S(f) = -\int f \log f$$

THEOREM: One has

$$\partial_t S(f_t) = \langle\sigma\rangle_{f_t} + \langle|\nabla_r \log\hat{\rho}|^2\rangle_{f_t} + \partial_t\langle r_1^2/2T_L + r_n^2/2T_R\rangle_{f_t}$$

3 terms:

Non-equilibrium, rearrangement, (time-) boundary

Fluctuations of entropy production

Gallavotti-Cohen, Kurchan, Lebowitz, Spohn

Here, only conjecture, because of lack of convergence proof

Consider scalar product

$$(f,g)_\rho \equiv \int \rho \bar{f} g$$

Let J = momentum reversal and set

$$A = \hat{\rho}^{-1} J$$

One has the symmetry property (time-reversal)

$$A^{-1} L^* A - L = \sigma, \quad A^* = A$$

with * the adjoint w.r.t. $(\cdot,\cdot)_\rho$

Consider random variable ``entropy production''

$$W(t) = \int_0^t d\tau\, \sigma(\xi_x(\tau))$$

and define

$$e(\lambda) \equiv - \lim_{t\to\infty} t^{-1} \log\langle e^{-\lambda W(t)}\rangle_\rho$$

Then, by symmetry, $e(\lambda) = e(1 - \lambda)$ and thus the Legendre transform satisfies

$$\hat{e}(x) - \hat{e}(-x) = -x \langle\sigma\rangle_\rho \qquad (*)$$

But we also have

$$\mathrm{Prob}(t^{-1}W(t) = x\langle\sigma\rangle_\rho) \approx \exp(-t\hat{e}(x))$$

CONJECTURE: The fluctuations of the entropy production satisfy (*)