

Non-equilibrium steady states for networks of springs

Work with C-A Pillet, L Rey-Bellet, M Hairer, N Cuneo, E Zabey

Restrict the discussion to

Heat Bath $\leftrightarrow$ Classical Hamiltonian System $\leftrightarrow$ Heat Bath

NOT quantum,

NO friction in the classical system,

NO stochastic driving (except for baths)

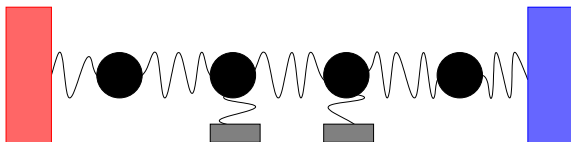
Typical questions:

- Existence of a steady state
- Uniqueness of the steady state (if it exists)
- Approach to the steady state

Today I want to concentrate on uniqueness

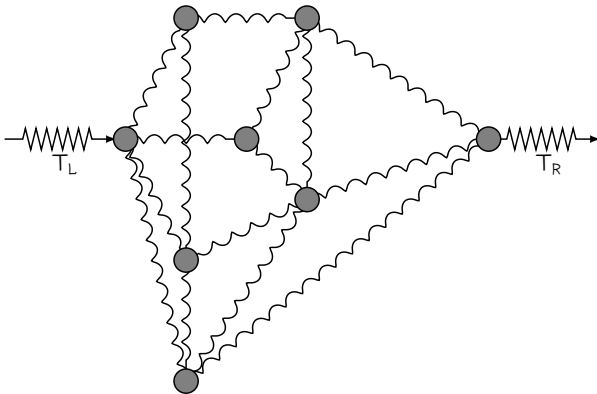
Models:

Chains of "springs"



Example of complicated graph

Here, just 2 heat baths



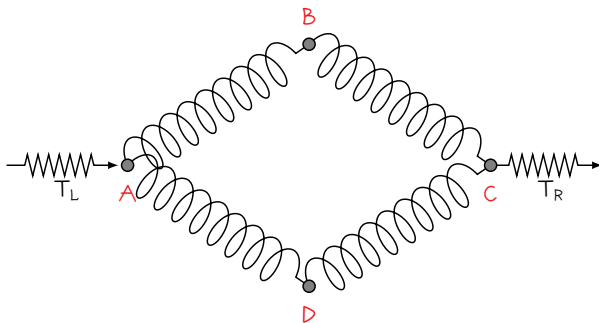
But let me start with the “heat baths”. Their role is to “forget” things about the state of the Hamiltonian system, and is the **only** source of dissipation in the study

Uniqueness

Absence of existence is caused by piling up of energy in the system

Absence of uniqueness is more related to absence of coupling, altogether

Example (JPE, E Zabey; C Maes, K Netocny,
and M Verschuere)



If the springs are harmonic and equal, then $p_B - p_D$ and $q_B - q_D$ evolve like a harmonic oscillator, decoupled from the rest of the system

Also non-unique in case of equilibrium

I will give now a review of what is known about this problem for general networks of springs

The main insight as of today can be summarized as follows

The steady state is unique if

either the network is "special" and then there is no restriction on the potentials

or the network is general and the potentials are "generic"

So what is "special" and what is "generic"?

In fact, one can look at mixtures of the two

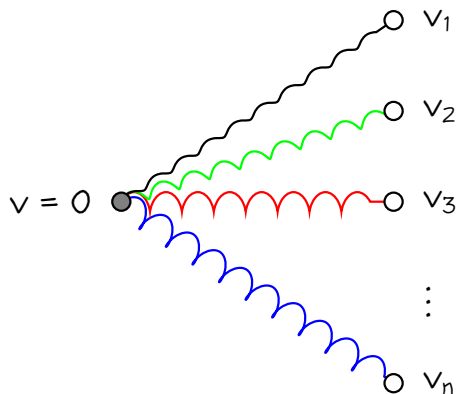
Getting Started

We consider a graph $\mathcal{G}$ made of masses (vertices) $\mathcal{V}$ and of springs (edges) $\mathcal{E}$

$$H = \sum_{v \in \mathcal{V}} \left(p_v^2 / 2 + U_v(q_v) \right) + \sum_{e \in \mathcal{E}} V_e(\delta q_e), \quad \delta q_e = q_{\text{from}} - q_{\text{to}}$$

Assume $V_e(x) = V_{-e}(-x) \neq 0$. All potentials are smooth

Some masses are attached to heat baths with temperatures $T_b > 0$ and coupling constant γ .



For simplicity I discuss the case when only $v = 0$ is attached to a bath and I let $\mathcal{E}_0$ be the edges which contain $v = 0$

The Hamiltonian

$$H = \sum_{v \in \mathcal{V}} (p_v^2/2 + U_v(q_v)) + \sum_{e \in \mathcal{E}} V_e(\delta q_e)$$

with the bath coupling, leads to the **Liouville operator**

$$L = X_0 + \gamma T \partial_{p_0}^2$$

with

$$X_0 = -\gamma p_0 \partial_{p_0} + \sum_{v \in \mathcal{V}} (p_v \partial_{q_v} - U'_v(q_v) \cdot \partial_{p_v}) - \sum_{e \in \mathcal{E}} V'_{u,v}(q_u - q_v) (\partial_{p_u} - \partial_{p_v})$$

It is then convenient to rewrite this

$\mathcal{E}_0$ the edges of links connected to the bath and $\mathcal{V}_0$ their other ends,

$$p_0 = p, q_0 = q$$

$$L = X_0 + \gamma T \partial_p^2$$

with (pinning potentials U are irrelevant here)

$$\begin{aligned} X_0 = & -\gamma p \partial_p + p \partial_q - u_0(q) \partial_p \\ & + \sum_{v \in \mathcal{V}_0} p_v \partial_{q_v} - \sum_{v \in \mathcal{V}_0} V'_{(0,v)}(q - q_v) \cdot (\partial_p - \partial_{p_v}) \\ & + \sum_{v \notin \mathcal{V}_0} p_v \partial_{q_v} - \sum_{e \notin \mathcal{E}_0} V'_e(\delta q_e) \cdot (\partial_p - \partial_{p_v}) \end{aligned}$$

where the top 2 lines deal with the masses connected to the heat bath

The uniqueness is shown by showing that the system is **controllable**,

the noise can drive the system from any phase space point to any other point in finite time. And this is shown using a **Hörmander condition**

Has been used since the paper with **Pillet** and **Rey-Bellet** but also by **Hairer & Mattingly** for the 2D Navier-Stokes, and in another variant by **Villani** for the Boltzmann equation

I will describe some new variants which are useful in our context

Task: show that "all" vector fields can be generated from the baths

Let $\mathcal{M}$ be the smallest set of vector fields that is closed under Lie brackets and multiplication by smooth functions and that contains

$$\partial_p \text{ and where one acts with } [\cdot, X_0]$$

To show:

For all $v \in \mathcal{V}$ the vector fields ∂_{p_v} and ∂_{q_v} are in $\mathcal{M}$

Sketch of method

First, $[\partial_p, X_0] = -\gamma \partial_p + \partial_q$, and therefore, since $\partial_p \in \mathcal{M}$, we find

$$\partial_q \in \mathcal{M}.$$

Moreover, since for all $v \in \mathcal{V}$ we have $[\partial_{p_v}, X_0] = \partial_{q_v}$, we have the implication

$$\partial_{p_v} \in \mathcal{M} \quad \Rightarrow \quad \partial_{q_v} \in \mathcal{M}$$

Thus, we need only show that the ∂_{p_v} are in $\mathcal{M}$

Since

$$[\partial_{\mathbf{q}}, X_0] = -u_0(\mathbf{q})\partial_{\mathbf{p}} - \sum_{e \in \mathcal{E}_0} V_e''(\mathbf{q} - \mathbf{q}_{to}) \cdot (\partial_{\mathbf{p}} - \partial_{\mathbf{p}_{to}}),$$

and $\partial_{\mathbf{p}} \in \mathcal{M}$, we obtain that

$$\sum_{v \in \mathcal{V}_0} V_{(0,v)}''(\mathbf{q} - \mathbf{q}_v) \partial_{\mathbf{p}_v} \in \mathcal{M}$$

Can we split this into $\partial_{\mathbf{p}_v} \in \mathcal{M}$ for each v and all $x = \mathbf{q} - \mathbf{q}_v$?

It is convenient to introduce the notation

$$g_e(x) = V_e''(x)$$

which is the second derivative of the coupling potential

With this notation, the inventory of vector fields in $\mathcal{M}$ we have found so far is then

$$\partial_p, \quad \partial_q, \quad \text{and} \quad \sum_{v \in \mathcal{V}_0} g_{(0,v)}(\mathbf{q} - \mathbf{q}_v) \partial_{p_v}$$

Starting from this, and taking further commutators (also with X_0) we want to show that each ∂_{p_v} is also in $\mathcal{M}$

QUESTION

Under what conditions do we have

$$\sum_{v \in \mathcal{V}_0} g_{(0,v)}(\mathbf{q} - \mathbf{q}_v) \partial_{p_v} \in \mathcal{M} \implies \partial_{p_v} \in \mathcal{M} \text{ for all } v \in \mathcal{V}_0 ?$$

Result 1: E, Pillet, Rey-Bellet

If

- only one spring is attached to bath (i.e. $|\mathcal{V}_0| = 1$)
- the dimension of system is 1
- g is strictly positive (i.e. the potential is strictly convex)

then

$$g_1(q - q_1)\partial_{p_1} \in \mathcal{M} \implies \partial_{p_1} \in \mathcal{M}$$

(Obvious, since $\mathcal{M}$ is closed under multiplication by scalar functions)

$\implies$ These chains can be handled because network is **special**

Result 2: E, Hairer, Rey-Bellet (to be written up)

The dimension of system is arbitrary

If

- topological condition on network (explained below)
- conditions on the potentials: for every $x \in \mathbb{R}^d$

$$\{D^\alpha \nabla V(x) : |\alpha| \leq \ell\}$$

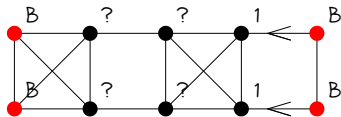
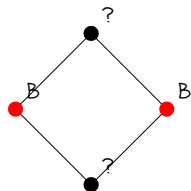
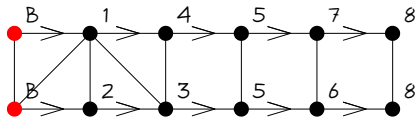
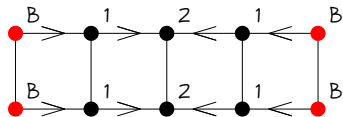
spans $\mathbb{R}^d$ (some sort of "eventual convexity")

then $D^\alpha \nabla V(x) \partial_{p_1} \in \mathcal{M}$ for all $\alpha \implies \partial_{p_1} \in \mathcal{M}$

Trick: The matrix

$$M_{ij}(x) = \sum_{1 \leq |\alpha| \leq \ell} (D^\alpha d_i V)(x) (D^\alpha d_j V)(x)$$

is invertible



No "already controlled" node controls more than one new node

⇒ Can be handled because network is special

Result 3: E, Cuneo (with some help by D. Sullivan, maybe never written up)

Basically no restriction on anything, but only a relatively abstract result

Assume for every edge e in the connection graph the potential is a **polynomial** of the form $V_e(x) = \sum a_{ej} x^j$

The set of coefficients for which the V_e are linearly dependent modulo translations ($\sum \gamma_e V_e(x - \tau_e) = 0$) for all $x \in \mathbb{R}^d$ is a semi-algebraic set $\mathcal{W}$. For any choice of coefficients in the **complement** of $\mathcal{W}$, controllability holds

So, generically controllable if $\deg V_e \geq 2n + 1$ when $|\mathcal{E}_0| = n$.

$\implies$ Holds because potentials are **generic**

Result 4: E, Cuneo More precise genericity

If the (second derivatives of the) potentials are pairwise unequal modulo translations, of degree ≥ 3 , then controllability holds

Harmonic potentials make problems

Technique: not only commutators with the ∂_p but also with ∂_{p_v} of the other side of the links

Main algebraic ingredient (with $e = (0, v)$):

$$\sum_{v \in \mathcal{V}_0} g_e(x_e) \partial_{p_v} \in \mathcal{M} \implies \sum_{v \in \mathcal{V}_0} g'_e(x_e) \partial_{p_v} \in \mathcal{M}$$

$$\sum_{v \in \mathcal{V}_0} g_e(x_e) \partial_{p_v} \in \mathcal{M} \implies \sum_{v \in \mathcal{V}_0} (x_e \cdot g_e(x_e))' \partial_{p_v} \in \mathcal{M}$$

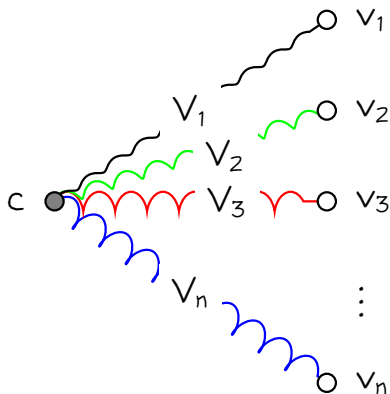
$\implies$ Holds because potentials are generic

Result 5: E, Cuneo

Restrictions on **topology** of network but not on potential
(1-D)

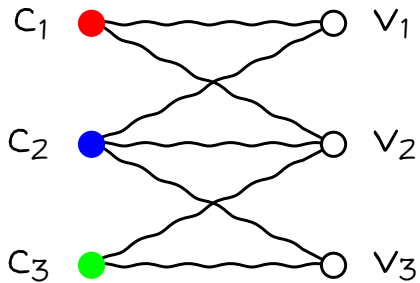
Assume set C of nodes is already known to control. Then any new v can be controlled if no other mass has the same connections to C

One can combine the **generic** and the **topological** conditions



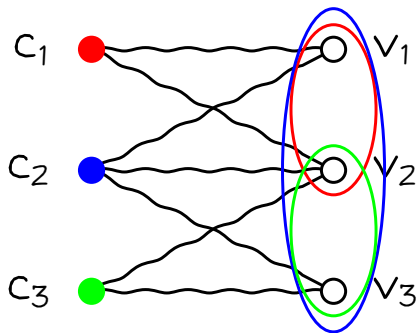
Pairwise inequivalent potentials:

One node can control all particles on the right



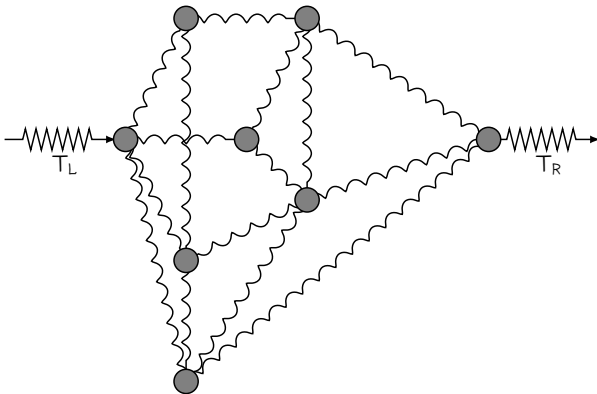
Purely topological example

Examples



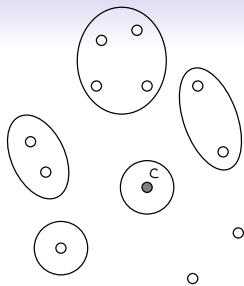
Purely topological example

Examples

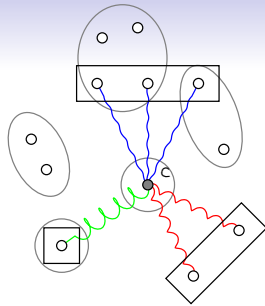


Is controllable !

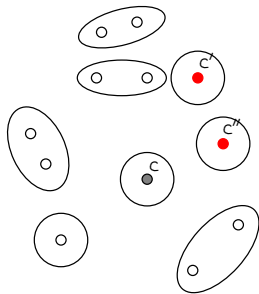
Examples



topological splitting



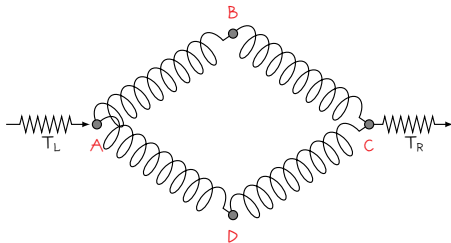
potential splitting



effect of topology and potentials

The future?

Try to get rid of as many conditions as possible. But **remember!** Not every network works. (And not all controllable networks are captured by our methods)



Analytic potentials?