The Frenkel-Kontorova model for almost-periodic environments of Fibonacci type

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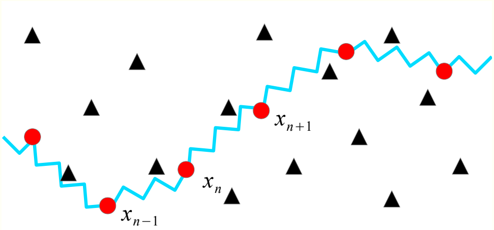
The physical problem



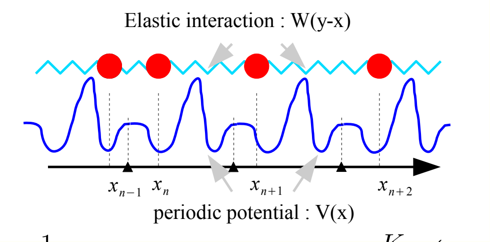
Consider the problem of arranging a chain of atoms or a long polymer (red spots) on a two-dimensional substrate possessing a quasi-crystal structure (black spots). Assume

- $x_n \in \mathbb{R}^d$ position of the nth atom
- Each atom interacts with its nearest neighbors
- $E(x_n, x_{n+1})$ = energy for the nth site = $W(x_{n+1} - x_n) + V(x_n)$
- $W(y - x)$: mutual internal interaction between atoms
- $V(x)$: external interaction with the substrate

Find a configuration of atoms with the lowest total energy

The mathematical problem

1. The original Frenkel-Kontorova model : $d = 1$ and $V(x)$ is periodic



$$W(y-x) := \frac{1}{2}|y-x-\lambda|^2, \qquad V(x) := \frac{K}{(2\pi)^2}\Big(1-\cos(2\pi x)\Big)$$

2. The periodic multi-dimensional Frenkel-Kontorova model: $\quad x_n \in \mathbb{R}^d$

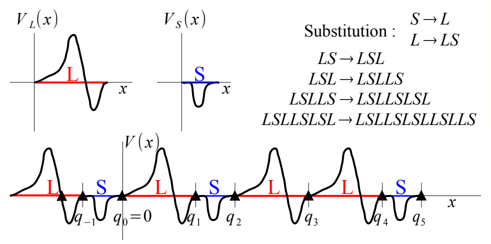
E is C^2 and periodic: $\quad E(x+1, y+1) = E(x,y)$

E is superlinear: $\quad \lim_{\|y-x\|\to+\infty} \frac{E(x,y)}{\|y-x\|} = +\infty$

E is twist: $\quad \sum_i \sum_j \frac{\partial^2 E}{\partial x_i \partial y_j} v_i v_j \leq -\alpha \sum_i v_i^2, \quad \alpha > 0$

The mathematical problem

3. The Frenkel-Kontorova model of Fibonacci type: $W(t) = \frac{1}{2}|t - \lambda|^2$



4. **Problem:** Let $E(x, y) = W(y - x) + V(x)$. Describe the set of configurations $\{x_n\}_{n \in \mathbb{Z}}$ with the lowest total energy

$$\text{“}E_{tot} = \sum_{n \in \mathbb{Z}} E(x_n, x_{n+1})\text{”}$$

or configurations which are **minimizing in the Aubry sense**

$$E(x_n, \dots, x_{n+k}) := \sum_{i=0}^{k-1} E(x_{n+i}, x_{n+i+1}) \le E(y_n, \dots, y_{n+k})$$

whenever $x_n = y_n$ and $x_{n+k} = y_{n+k}$, for all $n \in \mathbb{Z}$ and $k \ge 1$

Previous results

1. The original Frenkel-Kontorova model, (Aubry, 1985):
There exist minimizing configurations for any rotation number and every minimizing configuration admits a rotation number. The proof uses **the order of** $\mathbb{R}$.

2. The periodic multi-dimensional Frenkel-Kontorova, (Mather, 1990):
There exist minimizing configurations with a rotation vector as large as we want. The proof uses a new notion: **minimizing measures in the Mather sense**.

3. The Frenkel-Kontorova model of Fibonacci type, (Gambaudo - Guiraud - Petite, 2006): Same results as in the periodic case. Again the order of $\mathbb{R}$ is unavoidable. A general Fibonacci-Frenkel-Kontorova:

– let $\bar{\omega}$ be a **quasi-crystal** (A Delone set in $\mathbb{R}$ which is has uniform local complexity, is repetitive, and has uniform pattern distribution)
– let $\bar{V} : \mathbb{R} \to \mathbb{R}$ be a **pattern equivariant function**: there exists $R > 0$

$$\forall x, y \in \mathbb{R}, \quad B(0,R) \cap (\bar{\omega} - x) = B(0,R) \cap (\bar{\omega} - y) \Longrightarrow \bar{V}(x) = \bar{V}(y)$$

– $E(x_n, x_{n+1}) = W(x_{n+1} - x_n) + \bar{V}(x_n), \quad (W(t) = \frac{1}{2}|t - \lambda|^2)$

Problem and extension

Problem: Consider a Delone set $\bar\omega \subset \mathbb{R}^d$ which is repetive and has finite local complexity. Consider $\bar V : \mathbb{R}^d \to \mathbb{R}$ a pattern equivariant continuous potential. Define $E(x,y) = W(y-x) + \bar V(x)$

Does there always exist a minimizing configuration?

Partial answer: As soon as V is bounded and continuous, there always exists a one-sided minimizing configuration $\{x_n\}_{n\geq 0}$ starting at any point.

Extension: Let Ω be the hull of $\bar\omega$ then $(\Omega, \mathbb{R}^d)$ becomes a compact minimal system. Thanks to the equivariance of $\bar V$

$$\exists V : \Omega \to \mathbb{R},\ \forall x \in \mathbb{R}^d, \quad V(\bar\omega - x) = \bar V(x)$$

Define a "Lagrangian" $L(\omega, t) = W(t) + V(\omega)$ on $\Omega \times \mathbb{R}^d$. We say that $(\Omega, \mathbb{R}^d, L)$ is an **almost periodic interaction model**. More generally

- $(\Omega, \mathbb{R}^d)$ is compact minimal
- L is just supposed to be coersive: $\lim\limits_{R\to+\infty} \inf_{\|t\|\geq R,\ \omega\in\Omega} L(\omega,t) = +\infty$
- Each ω defines an interaction energy: $E_\omega(x,y) = L(\omega - x, y - x)$

An important observation

A minimizing configuration does not detect the lowest energy.

The ground energy

$$\bar{E} := \lim_{n \to +\infty} \inf_{x_0, \ldots, x_n \in \mathbb{R}^d} \frac{1}{n} E(x_0, \ldots, x_n)$$

– Modify E by adding a "linear coboundary":

$$E_\lambda(x, y) = E(x, y) - \langle \lambda, y - x \rangle$$

– Observe:

$\{x_n\}_{n \in \mathbb{Z}}$ is minimizing for E_λ $\iff$ $\{x_n\}_{n \in \mathbb{Z}}$ is minimizing for E

– But certainly $\lambda \mapsto \bar{E}(\lambda)$ is not a constant function.

Our objective: Find a stronger notion of configuration so that it detects the ground energy.

Calibrated configuration

Model: Let $(\Omega, \mathbb{R}^d, L)$ be an almost periodic interaction model of Lagrangian type $L : \Omega \times \mathbb{R}^d \to \mathbb{R}$.

calibrated sub-cocycle: Any function $\Phi : \Omega \times \mathbb{R}^d \to \mathbb{R}$ satisfying

$$\Phi(\omega, t) \leq L(\omega, t) - \bar{E}$$
$$\Phi(\omega, s+t) \leq \Phi(\omega, s) + \Phi(\omega - s, t)$$

In terms of the interaction family $E_\omega(x,y) = L(\omega - x, y - x)$ define

$$\Phi_\omega(x,y) = \Phi(\omega - x, y - x)$$

then in an equivalent way

$$\Phi_\omega(x,y) \leq E_\omega(x,y) - \bar{E}, \qquad \Phi_\omega(x,y) \leq \Phi_\omega(x,z) + \Phi_\omega(z,y)$$

Definition: A configuration $\{x_n\}_{n\in\mathbb{Z}}$ is **Φ-calibrated** (in the environment ω) if

$$\forall n \in \mathbb{Z},\ \forall k \geq 0, \quad E_\omega(x_n, \dots, x_{n+k}) - k\bar{E} = \Phi_\omega(x_n, x_{n+k})$$

Easy claim: A calibrated configuration is minimizing. (The converse is false in general).

Main Result

Mañé potential: The Mañé potential is a calibrated sub-cocycle:

$$\Phi(\omega,t) = \inf_{n\geq 1} \inf_{0=x_0,\ldots,x_n=t} \sum_{k=0}^{n-1} \big[L(\omega - x_k, x_{k+1}-x_k) - \bar{E}\big]$$
$$= \inf_{n\geq 1} \inf_{0=x_0,\ldots,x_n=t} E_\omega(x_0,\ldots,x_n) - n\bar{E}$$

(Φ is upper semicontinuous.)

Main result: Let $(\Omega, \mathbb{R}^d, L)$ be an almost periodic interaction model of Lagrangian type. Assume L is continuous and coersive. Then

– There exists $\omega \in \Omega$ such that E_ω admits a Φ-calibrated configuration $\{x_n\}_{n\in\mathbb{Z}}$. In addition $x_0 = 0$ and $\sup_{n\in\mathbb{Z}} \|x_{n+1}-x_n\| < +\infty$. Actually every $\omega \in \mathrm{Mather}(L)$ satisfies the above property.

– For a quasi-crystal in $d=1$, every E_ω admits a calibrated configuration (not necessarily passing through the origin). Actually $\mathrm{Mather}(L)$ is transverse to the action.

What is the Mather set?

Mather set: Mather(L)

Motivation: Choose $\bar{\omega} \in \Omega$ and choose a sequence of configurations of finite size $(x_0, \ldots, x_n)$ so that

$$\frac{1}{n} E_{\bar{\omega}}(x_0, \ldots, x_n) \to \bar{E}$$

Define $\mu_{\bar{\omega},n} := \frac{1}{n} \sum_{k=0}^{n-1} \delta(\bar{\omega} - x_k, x_{k+1} - x_k)$ on $\Omega \times \mathbb{R}^d$. Notice

$$\int f(\omega)\, d\mu_{\bar{\omega},n}(\omega,t) - \int f(\omega - t)\, d\mu_{\bar{\omega},n}(\omega,t) = \frac{1}{n}\Big[f(\bar{\omega} - x_0) - f(\bar{\omega} - x_n) \Big]$$

Holonomic measures: A probability measure μ on $\Omega \times \mathbb{R}^d$ is holonomic

$$\forall f \in C^0(\Omega), \quad \int f(\omega)\, d\mu(\omega,t) = \int f(\omega - t)\, d\mu(\omega,t)$$

Minimimizing measures: μ is minimizing if it is holonomic and

$$\int f d\mu = \inf \Big\{ \int L(\omega,t)\, d\nu(\omega,t) : \nu \text{ is holonomic} \Big\}$$

Mather set: $\mathrm{Mather}(L) := \bigcup_{\mu \text{ is minimizing}} \mathrm{supp}(\mu) =$ a compact set

Proof of the main result

Main result: For every $\omega \in \mathrm{Mather}(L)$ there exists a Φ-calibrated sequence $\{x_n\}_{n\in\mathbb{Z}}$ such that $x_0 = 0$ and

$$\Phi(\omega, x_n) = \sum_{k=0}^{n-1} \big[L(\omega - x_k, x_{k+1} - x_k) - \bar{E}\big]$$

Essentially: Prove $\quad \Phi(\omega, t) = L(\omega, t) - \bar{E} \quad$ on $\mathrm{Mather}(L)$

Technical part: To compute the ground energy in different ways

$$\begin{aligned} \bar{E} &= \min_{\mu \text{ is holonomic}} \int L(\omega,t)\, d\mu(\omega,t) \\ &= \sup_{u\in C^0(\Omega)} \ \inf_{\omega\in\Omega,\ t\in\mathbb{R}^d} \ \big[L(\omega,t) - u(\omega - t) + u(\omega)\big] \end{aligned}$$

Proof: Choose a family $u_\epsilon \in C^0(\Omega)$ such that

$$u_\epsilon(\omega - t) - u_\epsilon(\omega) \le L(\omega, t) - \bar{E} + \epsilon$$

Define a measurable sub-cocycle: $\quad U(\omega, t) = \limsup_{\epsilon\to 0}\ u_\epsilon(\omega - t) - u_\epsilon(\omega)$

$$U \le \Phi \le L - \bar{E} \quad \Longrightarrow \quad \Phi = L - \bar{E} \quad \text{on } \mathrm{Mather}(L)$$