Classification of calibrated configurations and effective potential for a quasiperiodic environment

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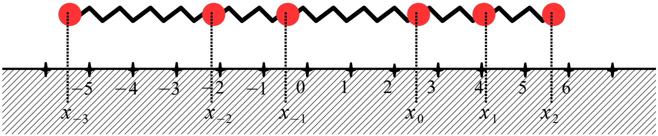
Summary

- I. **Position of the problem**
- II. Old and new results

I.1. The standard Frenkel-Kontorova model

Problem We consider the process of depositing a thin layer of a metallic gas over a substrate possessing a periodic structure like a crystal.



The black dots represent the atoms of the crystal, the red dots, the atoms of the gas. The atoms on the crystal are arranged periodically (of unit 1), the atoms of the gas undergo two forces :

- a mutual interaction between two neighbors
- a periodic external interaction with the substrate

I.2. Basic assumptions

The total energy We assume the substrate is infinite, we expect that the atoms of the gas are laid down monotonically in order to be indexed by $\mathbb{Z}$.

$$E_{tot} = \sum_{n \in \mathbb{Z}} W(x_{n+1} - x_n) + V(x_n)$$

The original Frenkel-Kontorova model

$$W(y-x) = \frac{1}{2}(y - x - \lambda)^2, \quad V(x) = \kappa(1 - \cos(2\pi x))$$

- W is a potential for an elastic force, λ is the distance between the atoms when they undergo no forces (the natural distance of a string at rest), V is a periodic force, κ is a coupling term.
- For κ large, the particles are pinned at the minimum of V,

$$\forall n \in \mathbb{Z},\ x_n \in \mathbb{Z}$$

- For small κ, the particles are elastically at rest

$$\forall n \in \mathbb{Z},\ x_n = n\lambda + x_0.$$

I.3. Main questions

Question We want to understand the set of ground configurations of the model : the set of the positions of the metallic atoms $(x_n)_{n\in\mathbb{Z}}$ at the lowest energy

$$\{\text{ ground configurations }\} = \arg\min_{(x_n)_{n\in\mathbb{Z}}} \sum_{n\in\mathbb{Z}} \big[W(x_{n+1}-x_n)+V(x_n)\big]$$

Frenkel-Kontorova there is a competition between the positions given by an arithmetic progression $x_n = n\lambda + x_0$ and positions given by the period of the substrate $x_n \in \mathbb{Z}$

Strategy

- Define the notion of ground configurations
- Define the notion of ground state (translation invariant periodic probabilities)
- Study the resilience of the model with respect to a small perturbation of the external potential

Remark There is a natural symmetry in the periodic case

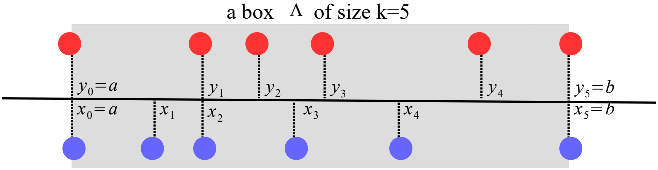
$$(x_n)_{n\in\mathbb{Z}} \text{ a ground configuration} \quad \Rightarrow \quad (x_n+1)_{n\in\mathbb{Z}} \text{ a ground configuration}$$

I.4. Ground configuration (weak sense)

Two notions of ground configurations

- (weak sense) minimizing configuration
- (strong sense) calibrated configuration

Weak sense $(x_n)_{n\in\mathbb{Z}}$ is said to be minimizing if



The blue configuration is minimizing

for every $\ell \in \mathbb{Z}$ and $k \geq 1$, for every other configuration $(y_n)_{n=\ell}^{n=\ell+k}$,

$$\text{if} \quad x_\ell = y_\ell \ \text{ and } \ x_{\ell+k} = y_{\ell+k} \quad \text{then}$$

$$\sum_{n=\ell}^{n=\ell+k-1} \big[W(x_{n+1}-x_n)+V(x_n)\big] \leq \sum_{n=\ell}^{n=\ell+k-1} \big[W(y_{n+1}-y_n)+V(y_n)\big]$$

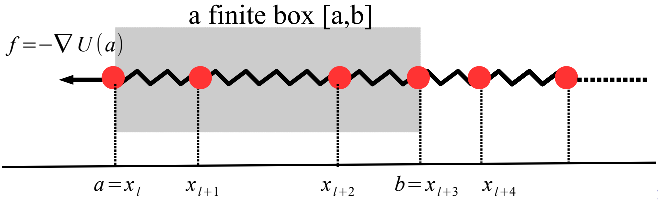
I.5. Ground configuration (strong sense)

Strong sense A configuration $(x_n)_{n\in\mathbb{Z}}$ is said to be calibrated if there exists an effective potential $U:\mathbb{R}\to\mathbb{R}$ that calibrates the configuration :

- U creates a force on the left hand side of any finite box $[a,b]$ so that, if the particles at the left hand side are erased and replaced by the effective force, the configuration stay unchanged
- the potential at the right hand side should count the sum of the energy of the box and the energy at the left hand size

$$\text{if} \quad x_\ell = a, \quad x_{\ell+k} = b \quad \text{then}$$

$$U(b) = U(a) + \sum_{n=\ell}^{n=\ell+k-1} \left[W(x_{n+1}-x_n) + V(x_n) - \bar{E}\right]$$



I.6. Effective potential : formal approach

Definition

- an effective potential $U : \mathbb{R} \to \mathbb{R}$ periodic

$$\begin{cases} \exists\, \bar{E} \quad \text{an effective energy} \\ \forall\, a < b,\ U(b) - U(a) \leq \big[W(b-a) + V(a) - \bar{E}\big] \\ \forall\, b,\ \exists\, a,\ U(b) - U(a) = \big[W(b-a) + V(a) - \bar{E}\big] \end{cases}$$

Remarks There are many names for U

- Griffiths, R.B., Chou, W. Phys. Rev. Lett. 56, 1929–1931 (1986) $\to$ effective potential
- Lions P. L., Papanicolaou G. C. and Varadhan S. R. (1987) $\to$ correctors
- Fathi A. “The Weak KAM Theorem in Lagrangian Dynamics” Cambridge (2016) $\to$ weak KAM solution

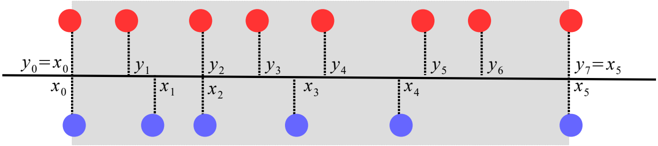
I.7. Effective potential : formal approach

Definition A configuration $(x_n)_{n\in\mathbb{Z}}$ is U-calibrated if for every $\ell \in \mathbb{Z}$, $k \geq 1$,

$$\sum_{n=\ell}^{\ell+k-1} \left[W(x_{n+1}-x_n)+V(x_n)-\bar{E}\right] = U(x_{\ell+k}) - U(x_\ell)$$

if $(y_n)_{n\in\mathbb{Z}}$ is another configuration so that $y_i = x_\ell$ and $y_j = x_{\ell+k}$ then

$$\sum_{n=\ell}^{\ell+k-1} \left[W(x_{n+1}-x_n)+V(x_n)-\bar{E}\right] \leq \sum_{n=i}^{j-1} \left[W(x_{n+1}-x_n)+V(x_n)-\bar{E}\right]$$



The blue configuration is calibrated

I.8. Mañé potential Φ

Remark

- A calibrated configuration is a minimizing configuration
- An effective potential may be difficult to construct ; calibration is observed through the difference $U(b) - U(a)$; an intermediate notion exists

Definition The Mañé potential is the relative energy barrier (with respect to a given effective energy $\bar{E}$) that a calibrated configuration should gain across a box

$$\Phi(a,b) = \inf_{k\geq 1} \inf_{a=x_0,\ldots,x_k=b} \sum_{n=0}^{k-1} \big[W(x_{n+1}-x_n) + V(x_n) - \bar{E}\big]$$

Definition A configuration $(x_n)_{n\in\mathbb{Z}}$ is Mañé calibrated if

$$\forall\, \ell \in \mathbb{Z},\ \forall\, k \geq 1,\ \sum_{n=\ell}^{\ell+k-1} \big[W(x_{n+1}-x_n) + V(x_n) - \bar{E}\big] = \Phi(x_\ell, x_{\ell+k})$$

I.9. Generalized Frenkel-Kontorova model

Recall

$$E(x,y) = W(y-x) + V(x) = \frac{1}{2}(y-x-\lambda)^2 + \kappa(1-\cos(2\pi x))$$

Hypotheses $E_\lambda(x,y) = E_0(x,y) - \lambda(y-x)$

- $E_0(x,y)$ is C^2 and uniformly Lipschitz on $|y-x|$
- $E_0(x+1,y+1) = E_0(x,y)$ (translation invariance)
- $\dfrac{\partial^2 E_0}{\partial x \partial y} \leq -\alpha < 0$ twist condition)
- $\lim_{R\to+\infty} \inf_{|y-x|\geq R} \dfrac{E_0(x,y)}{1+|y-x|} = +\infty$ (super linearity)

Remark The Frenkel Kontorova model is a model of unbounded spins with a periodic one-body interaction. It could be defined for $\mathbb{Z}^d$ lattices and for higher dimensional state space $\mathbb{R}^N$. Here

$$d = 1, \quad N = 1$$

I.10. Aubry-Mather theory

Remark A minimizing configuration $(x_n)_{n\in\mathbb{Z}}$ is critical in the sense

$$\partial_2 E(x_{n-1}, x_n) + \partial_1 E(x_n, x_{n+1}) = 0$$

The twist map The set of critical configuration is 2-dimensional. One introduces new variables

$$\begin{cases} p_n = -\partial_1 E(x_n, x_{n+1}) \\ p_{n+1} = \partial_2 (x_n, x_{n+1}) \end{cases}$$

The twist map is

$$F : \begin{bmatrix} x_n \mod 1 \\ p_n \end{bmatrix} \to \begin{bmatrix} x_{n+1} \mod 1 \\ p_{n+1} \end{bmatrix}$$

The Chirikov map For the Frenkel-Kontorova model

$$\begin{cases} x' = x + \lambda + p' \\ p' = p + 2\pi\kappa \sin(2\pi x) \end{cases}$$

Summary

- I. Position of the problem
- II. **Old and new results**

II.1. Summary

Notations $E(x,y) = W(y-x) - \lambda(y-x) + V(x)$

- V is periodic C^2 (old results) V is quasiperiodic (new results)
- W is C^2 uniformly strictly convex (twist and superlinearity conditions)

Problem We want to understand the set of ground configurations $(x_n)_{n\in\mathbb{Z}}$

$$\{ \text{ ground configurations } \} = \arg\min_{(x_n)_{n\in\mathbb{Z}}} \sum_{n\in\mathbb{Z}} E(x_n, x_{n+1})$$

either minimizing or U-calibrated

- U is continuous sublinear (periodic if V is periodic)

$$\limsup_{x\to\pm\infty} \frac{U(x)}{x} = 0$$

- there exists $\bar{E} \in \mathbb{R}$

$$\forall\, y \in \mathbb{R},\ U(y) + \bar{E} = \inf_{x\in\mathbb{R}} \big[U(x) + E(x,y)\big]$$

Remark The sublinearity condition insures the uniqueness of the effective energy

II.2. Effective potential and energy

Notation $E(x_0, x_1, \ldots, , x_n) = \sum_{k=0}^{n-1} E(x_k, x_{k+1})$

Easy result There is a natural candidate for the effective energy

$$\bar{E} = \lim_{n \to +\infty} \inf_{x_0, \ldots, x_n} \frac{1}{n} E(x_0, \ldots, x_n)$$

Definition (Lax-Oleinik) For every Lipschitz $U : \mathbb{R} \to \mathbb{R}$

$$T[U](y) = \min_{x \in \mathbb{R}} \{U(x) + E(x, y)\}$$

Theorem Assume V is periodic

- There exist $\lambda \in \mathbb{R}$ and a Lipschitz periodic function U solution of

$$T[U] = U + \lambda$$

- Necessarily $\lambda = \bar{E}$
- U may not be unique depending on the number of irreducible component of the Mather set

II.3. Calibrated configurations : Result

Recall A U-calibrated configuration $(x_n)_{n\in\mathbb{Z}} : \forall\, \ell \in \mathbb{Z},\ \forall\, k \geq 1$

$$E(x_\ell, \dots, x_{\ell+k}) - k\bar{E} = U(x_{\ell+k}) - U(x_\ell)$$

For any other configuration $(y_n)_{n\in\mathbb{Z}}$, if $i < j$, $x_\ell = y_i$, $x_j = y_{\ell+k}$

$$E(x_\ell, \dots, x_{\ell+k}) - k\bar{E} \leq E(y_i, \dots, y_j) - (j-i)\bar{E}$$

Theorem Assume V periodic. Let U be an effective potential. Then there exist U-calibrated configurations

Remark

- There is no need to assume W to be C^2 and strictly convex. W continuous and superlinear is enough to conclude
- there are cases in Frenkel-Kontorova, $|\lambda| \leq \frac{1}{40}\min(\kappa, 1)$, where all calibrated configurations belong to some/any cell $[N, N+1]$

II.4. Calibrated configurations : Algorithm

Algorithm

- take any x_0
- construct a backward orbit $(x_n)_{k=-\infty}^{k=0}$ which is half calibrated

$$x_{-k-1} \in \arg\min_{x\in\mathbb{R}}\{U(x) + E(x, x_{-k})\}$$

- choose $n \geq 0$, re-index $(y_k^n)_{k=-\infty}^{k=n}$ and shift by a multiple $p_n \in \mathbb{Z}$ of the period

$$y_k^n = x_{-n+k} + p_n \ \text{ so that } \ y_0^n \in [0,1], \quad \forall\, k \in]\!] -\infty, n]\!]$$

- take a converging subsequence $n \to +\infty$

II.5. Almost periodic setting

Definition The almost periodic setting

$$E(x,y) = \frac{1}{2}(y-x)^2 - \lambda(y-x) + V(x)$$
$$V(x) = \kappa_1(1-\cos(2\pi x)) + \kappa_2(1-\cos(2\pi\alpha x)), \quad \alpha \in \mathbb{R}\setminus\mathbb{Q}$$

Negative results For every $\kappa_1 > 0$, $\kappa_2 > 0$, there exists $C > 0$ such that if $|\lambda| \leq C\min(\kappa_1, \kappa_2, 1)$, then

- $\bar{E} = 0$ (the natural candidate)
- there is no minimizing configuration

II.6. Quasiperiodic setting

New modeling We imagine that the substrate is a quasicrystal : a crystal modified by impurities that are distributed with a low complexity (not i.i.d.) with patterns linearly repeated

Example : Fibonacci, symbolic setting

- we consider a substitution on symbols

$$\sigma : \begin{cases} 0 \mapsto 1 \\ 1 \mapsto 10 \end{cases} \qquad \sigma^2 : \begin{cases} 0 \mapsto 10 \\ 1 \mapsto 101 \end{cases}$$

- we construct a fixed bi-infinite point (for σ^2)

$$\omega = \cdots 10110\ 10\ 1 \mid 1\ 01\ 10101\ 1011010110101 \cdots$$
$$\omega = \cdots 10110101\ 101\ 1\ 0 \mid 1\ 01\ 10101\ 1011010110101 \cdots$$

II.7. Quasiperiodic setting : geometric setting

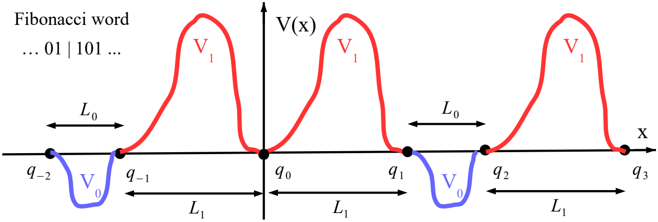
Example : Fibonacci, geometric setting

- we associate two lengths $0 < L_0 < L_1$; we distribute the impurities according the Fibonacci word

$$\omega = \cdots \omega_{-2}\omega_{-1}\mathrm{Id}\omega_0\omega_1\omega_2\cdots$$

$$q_0 = 0, \quad \forall\, k \geq 1,\ q_k = \sum_{\ell=1}^{k} L_{\omega_k}, \quad \forall\, k \leq -1,\ q_k = -\sum_{\ell=k}^{-1} L_{\omega_k}$$

- we define two potentials V_0, V_1 adapted to the impurities



II.8. Linear repetitivity

Definition A bi-infinit word $\omega = \cdots \omega_{-1} | \omega_0 \omega_1 \cdots$ is repetitive if for any admissible pattern $p = \omega_\ell \cdots \omega_{\ell+k}$ (a subword of ω), there is $M_p \geq 1$ so that for any n, the subword $\omega_{n+1} \cdots \omega_{n+M_p}$ of size M_p contains the pattern p

Definition A bi-infinite word is linearly repetitive if there exists $a > 0, b \geq 0$ such that

$$\forall \text{ pattern } p, \; M_p \leq a|p| + b$$

Lemma The Fibonacci fixed points are linearly repetitive

Remark There are other linearly repetitive sequences that are not a substitution : The Sturmian sequence, $\alpha \in (0,1)$

$$\omega_n = \lfloor (n+1)\alpha \rfloor - \lfloor n\alpha \rfloor \in \{0,1\}$$

II.9. Intermediate results

Additional assumptions

- E is non degenerate if

$$\inf_{x\in\mathbb{R}} E(x,x) > \bar{E}$$

- $E(x,y) = W(y-x) - \lambda(y-x) + V(x)$ is quasiperiodic if V is defined as before from a symbolic sequence $\omega \in \mathcal{A}^{\mathbb{Z}}$ in a finite alphabet that is linearly repetitive

Intermediate results

- if $(x_n)_{n\in\mathbb{Z}}$ is a calibrated configuration then it is monotone and unbounded of both sides
- $\exists\, 0 \le r \le R$

$$\forall\, n \in \mathbb{Z},\ r \le |x_{n+1} - x_n| \le R$$

- the rotation number exists

$$\lim_{n\to\pm\infty} \frac{x_n - x_0}{n} = \rho$$

- (if linearly repetitive) there exists a preferred ordering
  - positive ordering : all calibrated configuration are increasing
  - negative ordering : all calibrated configuration are decreasing

II.10. Main results

Theorem (Garibaldi, Petite, T.) Assume the non degeneracy condition and the quasiperiodic setting

- there exist calibrated configurations
- there exist effective potentials (of Lipschitz growth)

Assume the linear repetitiveness condition.

- There are 3 (non empty) types of effective potentials U. (Assume positive ordering for ibstance)
  - Type I :

$$\lim_{x \to \pm\infty} \frac{U(x)}{x} = 0$$

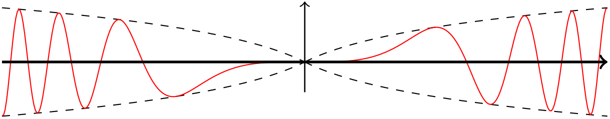
  - Type II :

$$\limsup_{x \to +\infty} \frac{U(x)}{|x|} \leq -\gamma, \quad \liminf_{x \to -\infty} \frac{U(x)}{|x|} \geq \gamma$$

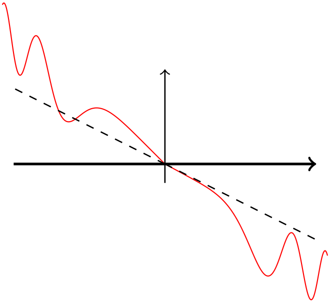
  - Type III (mixed type) :

$$\limsup_{x \to +\infty} \frac{U(x)}{|x|} \leq -\gamma, \quad \lim_{x \to -\infty} \frac{U(x)}{|x|} = 0$$

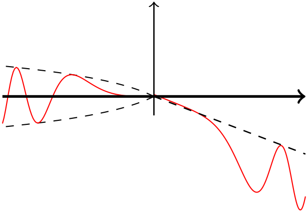
II.11. Main results



Sublinear growth at $\pm\infty$.



negative linear growth at $\pm\infty$



Sublinear growth at $-\infty$
negative linear growth at $+\infty$

Thank you