

Discommensuration Theory and Shadowing in Frenkel-Kontorova Models

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Dedicated to Serge Aubry on the occasion of his 60th birthday

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Abstract

We prove that if the minimum energy advancing discommensuration of mean spacing p/q for a Frenkel-Kontorova chain is unique up to translations and has phonon gap then all minimum energy states with mean spacing ω just above p/q are approximated exponentially well in $q\omega - p$ by concatenations of advancing p/q discommensuration.

1 Introduction

Aubry's theory of minimum energy states for Frenkel-Kontorova models is a beautiful body of work that has greatly enhanced understanding of how structure is determined in the solid state and played a key role in the interplay between condensed matter physics and dynamical systems theory and in our careers.

Here we treat one aspect of Frenkel-Kontorova models where dynamical systems ideas can add some extra insight. In [A], Aubry stated that “a configuration with atomic mean distance $l = [\frac{2ar}{s}] + \delta l$ ($\delta l > 0$) can be considered as a commensurate configuration with $\frac{s\delta l}{2a}$ equidistant advanced phase defects per atom which are then at distance $\frac{2a}{s\delta l}$ ” (where $2a$ is the period of the potential and r, s are integers). This point of view had also been expressed in [Mc], where the term “discommensuration” was introduced. It has become very fruitful, e.g. [Gr, FBG]. It is not clear, however, whether a complete justification has ever been provided.

Let us review the mathematical results of which we are aware in this direction. Firstly, by Aubry's theory of minimum energy states [AID], any minimum energy

state can be obtained as a limit in product topology of some sequence of minimum energy states with mean spacing converging to the given one; but product topology means only pointwise convergence, so that is a very weak result. Secondly, following [AIDA], Aubry had an idea that minimum energy states could be approximated exponentially well in δl by “arrays of discommensurations” (private communication); our memory is that there was some correspondence with Mather on this subject, but that there were problems with the proposed proof. Instead, in [AGARQ], Aubry developed a third approach: minimum energy states were decomposed into an exact superposition of translates of a single discommensuration-like profile; this profile, however, is not necessarily a minimum energy (nor even equilibrium) state itself.

Nevertheless, the idea of exponentially good approximation of minimum energy states by an array of discommensurations is good, so as a tribute to Aubry we have developed a precise statement and proof of such a result.

We present everything in solid-state physics language but translate into dynamical systems terminology where appropriate. The case we treat is the generic one where there is a unique (up to translation) minimum energy state of a given rational mean spacing (rotation number) p/q , it has phonon gap (is hyperbolic), and it has a unique (up to translation) advancing minimum energy discommensuration which also has phonon gap (transverse intersection of stable and unstable manifolds). The proof is via the dynamical systems theory of “shadowing”. The same can be done for a retreating discommensuration.

We recall necessary background results, then state and prove our result, and conclude with some remarks.

2 Necessary background

2.1 Frenkel-Kontorova models

A Frenkel-Kontorova model can be viewed as a doubly infinite one-dimensional chain of identical classical particles with convex nearest neighbour interaction, subject to a spatially periodic potential (whose period we scale to 1). More generally, the potential energy of the chain is the formal sum

$$H(\mathbf{x}) = \sum_{n \in \mathbb{Z}} h(x_n, x_{n+1}) , \quad (1)$$

where $x_n \in \mathbb{R}$ denotes the position of particle n , $\mathbf{x}$ denotes the state $(x_n)_{n \in \mathbb{Z}}$, and the function $h : \mathbb{R}^2 \rightarrow \mathbb{R}$ is C^2 and satisfies $h(x+1, x'+1) = h(x, x')$ and $h_{12} \leq -b$ for some $b > 0$ (subscript i on a function denotes partial derivative with respect to the i^{th} argument). The simplest case is $h(x, x') = W(x' - x) + V(x)$, with V a

periodic on-site potential of period 1: $V(x+1) = V(x)$, and W a strictly convex interaction potential between (nearest) neighbours: $W''(\xi) \geq b$. The potential energy of the chain is typically infinite but its gradient and the equilibria are well-defined.

Aubry was the first of whom we are aware to realise that there is a direct connection between a Frenkel-Kontorova model and an associated dynamical system [AA]. Specifically, the equilibrium states $h_2(x_{n-1}, x_n) + h_1(x_n, x_{n+1}) = 0$ of a Frenkel-Kontorova model are in 1-1 correspondence with orbits of an associated area-preserving twist map $f : (x, y) \mapsto (x', y')$ of the cylinder $\mathbb{T} \times \mathbb{R}$, defined implicitly by $y' = h_2(x, x')$, $y = -h_1(x, x')$. It is more convenient, however, to use the equivalent map $g : (x_{n-1}, x_n) \mapsto (x_n, x_{n+1})$ on the cylinder $\mathbb{R}^2/T$ where $T(x, x') = (x+1, x'+1)$. We measure the size of displacements (ξ, ξ') on the cylinder by $\max(|\xi|, |\xi'|)$.

2.2 Minimum energy states

Aubry defined a state $\mathbf{x}$ to have *minimum energy* if for all $M < N$ it (globally) minimises

$$W_{MN} = \sum_{n=M}^{N-1} h(x_n, x_{n+1}),$$

subject to x_M and x_N fixed.

A state $\mathbf{x}$ can be represented by a piecewise affine curve connecting the points $(n, x_n)_{n \in \mathbb{Z}}$ in order in the plane, called an *Aubry diagram*. Aubry proved that the graphs of two minimum energy states in the Aubry diagram cross at most once (*Aubry's fundamental lemma* [AID]). From this and invariance under the translations T_{pq} ,

$$(T_{pq}\mathbf{x})_n = x_{n+q} - p, \quad p, q \in \mathbb{Z}, \quad (2)$$

he proved that every minimum energy state $\mathbf{x}$ has a *mean spacing*

$$\rho = \lim_{M \rightarrow -\infty, N \rightarrow \infty} \frac{x_N - x_M}{N - M}.$$

In fact,

$$\text{floor}((n-m)\rho) < x_n - x_m < \text{ceil}((n-m)\rho) \text{ for all } m < n, \quad (3)$$

where $\text{floor}(x)$ is the greatest integer less than x and $\text{ceil}(x)$ is the least integer greater than x (this was proved in [MS] and in our opinion a uniform bound on $(x_n - x_m) - (n-m)\rho$ like this is a necessary step for a full proof of Aubry's classification of minimum energy states, as was done in [MS]).

Aubry proved there is a minimum energy state for each mean spacing ω [AID]. In the rational case, $\omega = p/q$ in lowest terms, there is a periodic minimum energy state with $x_{n+q} = x_n + p$ for all n (we say it has *type* (p, q)). The set $A_{p/q}$ of minimum energy states of type (p, q) is totally ordered in the partial order $\mathbf{x} \leq \mathbf{y}$ defined by $x_n \leq y_n$ for all $n \in \mathbb{Z}$. It is also closed (in product topology, but since the space of sequences of type (p, q) is finite-dimensional, it is also closed in uniform topology). If $\mathbf{L} < \mathbf{R}$ are two states in $A_{p/q}$ such that there is no $\mathbf{x} \in A_{p/q}$ with $\mathbf{L} < \mathbf{x} < \mathbf{R}$ we say $[\mathbf{L}, \mathbf{R}]$ is a *gap* in $A_{p/q}$. If $[\mathbf{L}, \mathbf{R}]$ is a gap in $A_{p/q}$ there is a minimum energy *advancing discommensuration* $\mathbf{v}$ with $L_n < v_n < R_n$ for all $n \in \mathbb{Z}$, $\mathbf{v} < T_{pq}\mathbf{v}$ and $v_n \rightarrow L_n$ as $n \rightarrow -\infty$, $v_n \rightarrow R_n$ as $n \rightarrow +\infty$. Similarly there is a *retreating discommensuration*, traversing the gap in the other direction. Denoting by $A_{p/q+}$ and $A_{p/q-}$ the sets of respectively advancing and retreating discommensurations of mean spacing p/q , and $A'_{p/q\pm}$ their unions with $A_{p/q}$, $A'_{p/q\pm}$ are totally ordered and closed (in product topology).

In the irrational case, we separate the set A'_ω of minimum energy states of mean spacing ω into the union of its recurrent ones and non-recurrent ones ($\mathbf{x}$ is *recurrent* if there exist sequences $n_k \rightarrow \infty$ and m_k such that $(x_{n_k} - m_k, x_{n_k+1} - m_k) \rightarrow (x_0, x_1)$ as $k \rightarrow \infty$). The set A_ω of recurrent minimum energy states of mean spacing ω is totally ordered and closed and is either a curve or a Cantor set. If A_ω is a curve then there are no non-recurrent ones, so $A'_\omega = A_\omega$. In the case that A_ω is a Cantor set, there are possibly some non-recurrent states in its gaps, but A'_ω is still totally ordered and closed.

Some of these results were also proved by Mather (starting in [Mat] independently of Aubry), so the subject is often called *Aubry-Mather theory* (for a review, see [Gol  ]). Corresponding to A_ω etc. we denote the invariant sets for the associated map g by M_ω etc.

2.3 Phonon gap

A configuration $\mathbf{x} \in \mathbb{R}^\mathbb{Z}$ is said to have *phonon gap* if the second derivative D^2H has bounded inverse in ℓ_2 -norm. The value of the phonon gap can be defined to be $\|D^2H^{-1}\|_2^{-1}$.

We proved that phonon gap for an equilibrium state (or set of them) is equivalent to uniform hyperbolicity for the corresponding invariant set of the associated twist map [AMB]. In particular, periodic equilibrium states whose corresponding orbit is hyperbolic have phonon gap, and if an equilibrium $\mathbf{x}$ has phonon gap then the Green function $\mathbf{G}$ for the linearised response to an infinitesimal force at $n = 0$ decays exponentially with uniform exponential bounds $|G_n| \leq C_0 \mu_0^{-|n|}$ for some $\mu_0 > 1$ and $C_0 > 0$. If μ is the supremum of μ_0 such that there is an exponential bound of this form then $\xi = 1/\log \mu$ is called the *coherence length* of $\mathbf{x}$.

It follows by homotopy that all equilibrium states $\mathbf{y}$ asymptotic to $\mathbf{x}$ to the right

(or left) converge to $\mathbf{x}$ with uniform exponential bounds of the form $|y_n - x_n| \leq C\mu_0^{\mp n}|y_0 - x_0|$ for $n > 0$ (respectively $n < 0$), for some C slightly larger than C_0 (starting with $|y_0 - x_0|$ small enough). The case of interest for this paper is when $\mathbf{x}$ is periodic, say of type (p, q) . In this case the supremum μ is attained and the above result (with $\mu_0 = \mu$) can be proved by converting to the associated dynamical system g : it becomes a question of the approach of orbits to a hyperbolic fixed point of g^q , which is asymptotically geometric with contraction factor equal to the modulus of the eigenvalue of Dg^q inside the unit circle. By the approach of [AMB] connecting hyperbolicity of g to decay of Green functions, this is μ^{-q} .

It also follows from [AMB] that a state with phonon gap is unique in some neighbourhood in uniform topology. More precisely, if A is a set of equilibrium states with phonon gap at least some $K > 0$ and whose associated invariant set on the cylinder is bounded, then there exists $\delta > 0$ such that if $\mathbf{x} \in A$ and $\mathbf{y}$ is an equilibrium state with $|y_n - x_n| < \delta$ for all $n \in \mathbb{Z}$ then $\mathbf{y} = \mathbf{x}$. This can be proved by establishing contraction of the map $\mathbf{y} \mapsto \mathbf{y} - D^2W^{-1}DW(\mathbf{y})$ on a δ -neighbourhood of $\mathbf{x}$.

We also proved that the phonon gap is continuous in Hausdorff topology on the orbits of the associated map [BM].

2.4 Shadowing

Let $\mathbf{w} \in \mathbb{R}^{\mathbb{Z}}$ be a *concatenation* of segments of equilibrium states $\mathbf{v}^k, k \in \mathbb{Z}$, of a Frenkel-Kontorova model, i.e. there exists an increasing sequence of integers n_k such that

$$w_n = v_n^k \text{ for } n = n_k + 1, \dots, n_{k+1}.$$

We define the *jumps* in $\mathbf{w}$ to be the 2D vectors $j^k = (v_{n_k}^k - v_{n_k}^{k-1}, v_{n_{k+1}}^k - v_{n_{k+1}}^{k-1})$. See Figure 1. We measure the size of a jump by $\max(|v_{n_k}^k - v_{n_k}^{k-1}|, |v_{n_{k+1}}^k - v_{n_{k+1}}^{k-1}|)$. We let $j(\mathbf{w})$ be the supremum of the jump sizes.

A translation of the shadowing theorem of Anosov and Bowen (e.g. [KH]) from dynamical systems theory into solid-state physics terminology yields:

Theorem 2.1. *If the $\mathbf{v}^k, k \in \mathbb{Z}$ all have phonon gap at least some $K > 0$ and lie in a bounded set when mapped to the cylinder then there exist $\delta > 0$ and $\kappa > 0$ such that if $j(\mathbf{w}) < \delta/\kappa$ there is an equilibrium state within $\kappa j(\mathbf{w})$ of $\mathbf{w}$ and it is unique within δ of $\mathbf{w}$.*

This can be proved for example by converting Palmer's proof [Pal] from first order to second order recurrence relations.

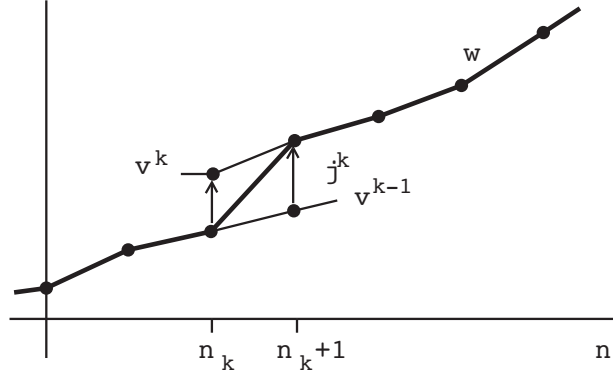


Figure 1: An Aubry diagram showing the jump from state $\mathbf{v}^{k-1}$ to $\mathbf{v}^k$ at $n = n_k$.

3 The result and its proof

We will approximate any minimum energy state of mean spacing just above a given rational p/q by a concatenation of segments of translates of an advancing minimum energy discommensuration of mean spacing p/q if the latter is unique up to translation and has phonon gap. These conditions are satisfied generically, so are not big restrictions. The rational p/q is fixed throughout and the interest is on how good the approximation can be made as a function of $\omega - p/q$.

Here is our result.

Theorem 3.1. *Suppose $A_{p/q+}$ is generated by a single (advancing discommensuration) state $\mathbf{v}$ and that it has phonon gap. Then: (i) $A_{p/q}$ is generated by a single (periodic) state $\mathbf{u}$ and it has finite coherence length $\xi < \infty$; (ii) there are constants $\varepsilon > 0, C', C''$ such that for all $\omega \in (p/q, p/q + \varepsilon)$ and all $\mathbf{y} \in A'_\omega$ there exists a concatenation $\mathbf{w}$ of segments of translates of $\mathbf{v}$ with jumps of size at most $C' \exp -\frac{1}{2\xi(q\omega-p)}$ and within $C'' \exp -\frac{1}{2\xi(q\omega-p)}$ of $\mathbf{y}$.*

Proof. (i) In each gap of $A_{p/q}$, as recalled in subsection 2.2, Aubry proved there is at least one advancing discommensuration. So if $A_{p/q+}$ is generated by a single discommensuration $\mathbf{v}$ then up to translations there is only one gap in $A_{p/q}$. Since $\mathbf{v}$ is assumed to have phonon gap, the periodic states to which it is asymptotic must also have phonon gap, and hence are isolated in $A_{p/q}$. So $A_{p/q}$ is generated by a single state we denote by $\mathbf{u}$, and it has phonon gap. It follows as in subsection 2.3 that $\mathbf{u}$ has finite coherence length, which we denote by ξ .

(ii) In the Aubry diagram, the graphs of $\mathbf{u}$, $\mathbf{v}$ and their translates form a lamination of the plane (see Figure 2). The closest translate of $\mathbf{u}$ above $\mathbf{u}$ is $T_{p',q'}\mathbf{u}$

where p'/q' is the upper Farey neighbour of p/q (the last convergent from the continued fraction expansion of p/q with $p'/q' > p/q$). The closest translate of $\mathbf{v}$ above $\mathbf{u}$ is $T_{pq}\mathbf{v}$.

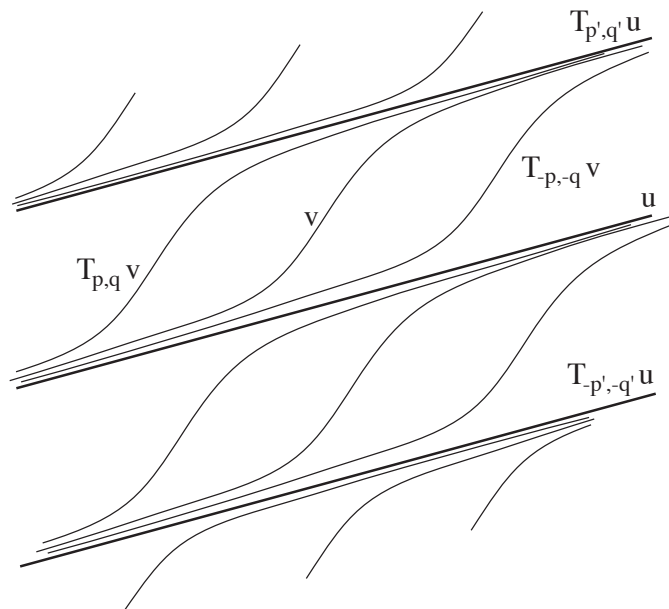


Figure 2: An Aubry diagram illustrating that the states in $A'_{p/q+}$ form a lamination of the plane (to simplify, we draw the graphs of $\mathbf{u}$ and its translates as straight lines and of $\mathbf{v}$ and its translates as smooth curves, rather than piecewise affine).

Given $\omega > p/q$ and $\mathbf{y} \in A'_\omega$, the graph of $\mathbf{y}$ crosses each of those of $\mathbf{u}$, $\mathbf{v}$ and their translates precisely once (and upwards), by Aubry's fundamental lemma.

Let $\delta > 0$ be such that we have the shadowing theorem for $A'_{p/q}$, and less than half the minimum distance between $\mathbf{u}$ and $T_{p'q'}\mathbf{u}$. Make a neighbourhood U of $\mathbf{u}$ bounded by segments of $\mathbf{v}$ and its translates, repeated with period q , within δ of $\mathbf{u}$. Specifically, let $\mathbf{v}^+ = \mathbf{v}$ and $\mathbf{v}^- = T_{kp-p',kq-q'}\mathbf{v}$ for some $k \in \mathbb{Z}$ (whose choice is irrelevant except for drawing figures) and choose segments $\mathbf{v}^\pm$ of length q (i.e. containing q successive atoms) within δ of $\mathbf{u}$, define $\mathbf{u}^\pm$ by extending them periodically using T_{pq} and define U as the region between $\mathbf{u}^\pm$ (see Figure 3).

Since $\mathbf{y}$ crosses each translate of $\mathbf{u}$ and $\mathbf{v}$ precisely once and upwards, $\mathbf{y}$ enters U from below and leaves U from above, and then crosses the gap between U and its translate $T_{p'q'}U$, and so on.

Lemma 3.2. *There exists J independent of ω such that the time P that y spends in U (or any translate) is at least $\frac{1}{q\omega-p} - J$.*

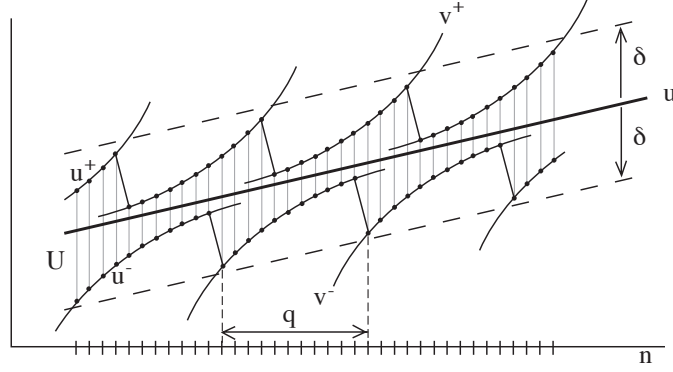


Figure 3: The neighbourhood U of $\mathbf{u}$ bounded by $\mathbf{u}^\pm$, made by repeating periodically segments of length q of $\mathbf{v}^\pm$ contained within δ of $\mathbf{u}$.

Proof. We use synonymously the terms “time” and “length” of a segment of $\mathbf{y}$ between crossings with two other states to mean the number of atoms of the segment; if a crossing happens at an atom we count it as half.

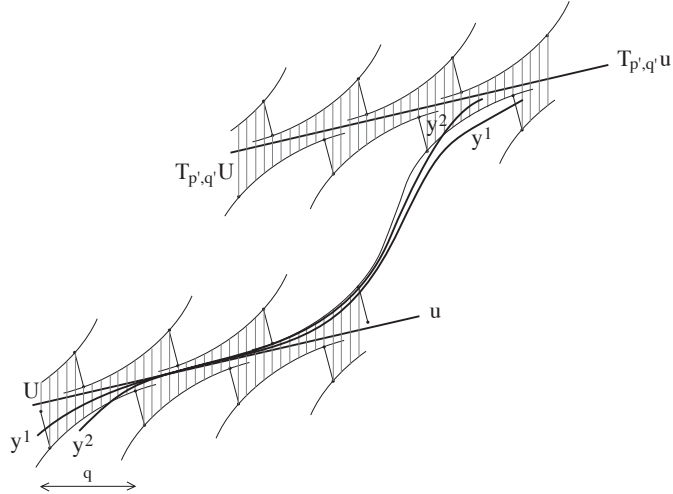


Figure 4: An Aubry diagram to show that if two segments of $\mathbf{y}$ between entries to successive translates of U differ in length by more than q then their graphs cross.

The lengths of segments of $\mathbf{y}$ between entries to successive translates of U differ by at most q , else translate two such segments to start in U and so that the longer one starts to the left of the shorter one but within q of it, then the segments would be forced to cross (see Figure 4), contradicting $\mathbf{y}$ being minimising. Thus the mean interval between entries of $\mathbf{y}$ to successive translates of U exists; furthermore it

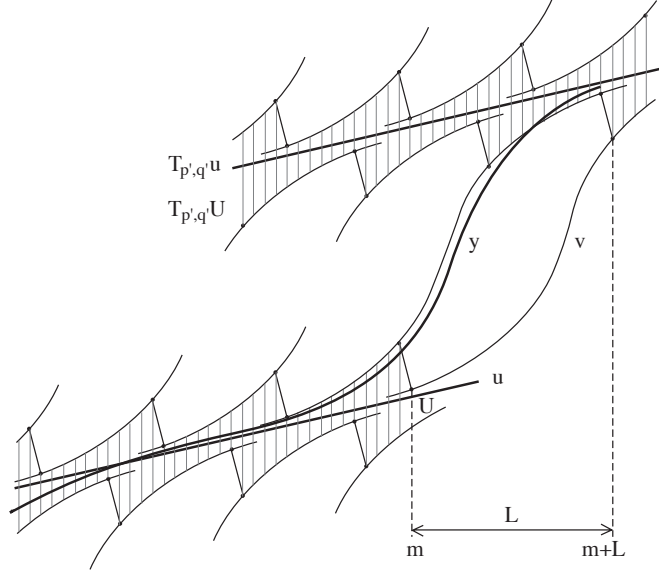


Figure 5: The length of a segment of $\mathbf{y}$ between exit of U and entry into $T_{p',q}U$ is at most $1 + L$ where L is the length of the indicated segment of $\mathbf{v}$.

is $\frac{1}{q\omega - p}$, else $\mathbf{y}$ would have a different mean spacing from ω . Because $\mathbf{y}$ crosses each translate of $\mathbf{v}$ precisely once and upwards, the intervals between exiting a translate of U and entering the next one are bounded by one plus the length L of the segment $v_m, \dots, v_{m+L}$ of $\mathbf{v}$ indicated in Figure 5. Hence the result, with $J = q + L + 1$. $\square$

Now choose $\delta' \in (0, \delta]$ so that the distance between $\mathbf{v}$ and $T_{pq}\mathbf{v}$ for $n = m, \dots, m + L - 1$ exceeds $2\delta'$. So there is an “island” which is avoided by all states which remain within δ' of the union of the translates of $\mathbf{v}$ (see Figure 6).

Lemma 3.3. *There exists $\varepsilon > 0$ such that the projection to the cylinder of every minimum energy state of mean spacing in $(p/q, p/q + \varepsilon)$ lies within δ' of $M_{p/q+}$.*

Proof. If not, there are sequences $\omega_k \rightarrow p/q +$ as $k \rightarrow \infty$, $\mathbf{y}^k \in A'_{\omega_k}$ and $n_k \in \mathbb{Z}$ such that $(\mathbf{y}^k_{n_k}, \mathbf{y}^k_{n_k+1})/T$ is not in the δ' -neighbourhood of $M_{p/q+}$. These points lie in a bounded subset of the cylinder because of (3), so have a convergent subsequence with a limit point (z_0, z_1) not in the δ' -neighbourhood. Being a limit of minimum energy states (in product topology) with mean spacing converging to $p/q +$, the orbit of (z_0, z_1) is in $M'_{p/q+}$ by Aubry’s theory, so is in the δ' -neighbourhood, which is a contradiction. $\square$

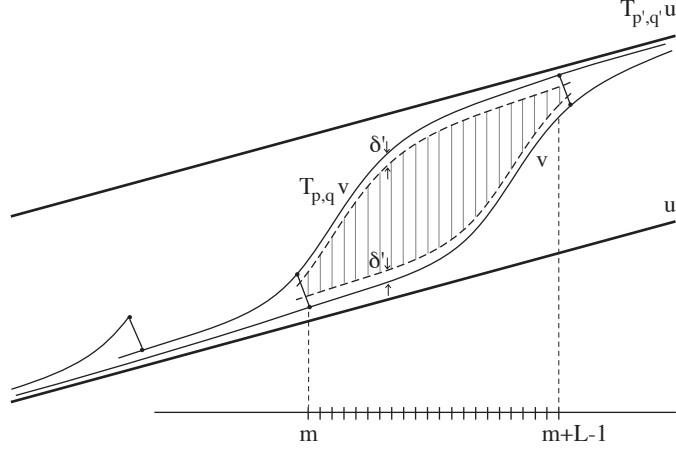


Figure 6: An “island” between $\mathbf{v}$ and $T_{pq}\mathbf{v}$, avoided by states within δ' of $A_{p/q+}$.

So, given $\omega \in (p/q, p/q + \varepsilon)$ and $\mathbf{y} \in A'_\omega$, $\mathbf{y}$ can not cross the island nor any of its translates. Thus for each gap in $A_{p/q}$, $\mathbf{y}$ follows within δ' a precise sequence from $A_{p/q+}$, say $\mathbf{D}$ between U and $T_{p'q'}U$ (Figure 7).

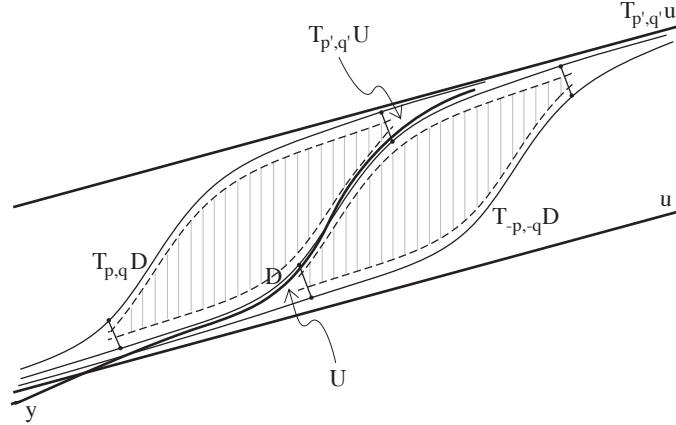


Figure 7: The state $\mathbf{y}$ follows one translate $\mathbf{D}$ of $\mathbf{v}$ within δ' across the given gap in $A_{p/q}$.

Similarly, $\mathbf{y}$ follows a specific discommensuration $\mathbf{D}'$ within δ' between $T_{-p',-q'}U$ and U .

To make our concatenation $\mathbf{w}$ of discommensurations approximating $\mathbf{y}$, we need to choose where to switch from $\mathbf{D}'$ to $\mathbf{D}$. The most natural choice might be the place where $\mathbf{y}$ crosses $A_{p/q}$, but to make sure the jumps are exponentially

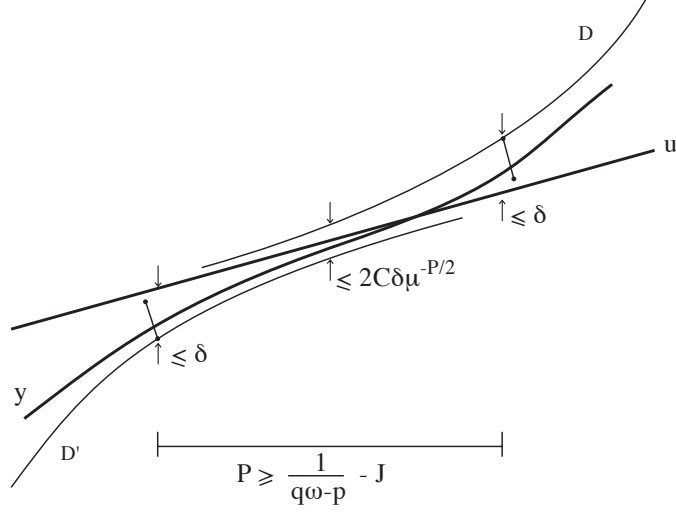


Figure 8: Halfway between entry and exit of $\mathbf{y}$ in/out of U , the chosen discommensurations $\mathbf{D}$, $\mathbf{D}'$ are within $C\delta\mu^{-P/2}$ of $\mathbf{u}$, with $P \geq \frac{1}{q\omega-p} - J$.

small (indeed, of the order anticipated in [A]) we make a different choice. We jump halfway between the entry and exit of $\mathbf{y}$ in and out of the neighbourhood U of the periodic state $\mathbf{u}$. By the result quoted in subsection 2.3, $\mathbf{D}'$ approaches $\mathbf{u}$ and $\mathbf{D}$ leaves $\mathbf{u}$ with exponential bounds of the form $C\delta\mu^{\pm n}$ with n measured from the entry or exit (see Figure 8). Thus halfway in between entry and exit, the distance between the two bounding discommensurations is at most $2C\delta\mu^{-P/2}$, where P is the number of atoms between entry and exit. So by Lemma 3.2, the jumps between discommensurations halfway between entry and exit have size at most $C'\mu^{-\frac{1}{2(q\omega-p)}}$ with $C' = 2C\delta\mu^{J/2}$.

By the shadowing theorem 2.1, it follows that there is a true equilibrium state $\mathbf{z}$ within $\kappa C'\mu^{-\frac{1}{2(q\omega-p)}}$ of the concatenation $\mathbf{w}$ of discommensurations, and that it is unique within δ of $\mathbf{w}$. By construction of $\mathbf{w}$, however, $\mathbf{y}$ is an equilibrium state within δ of $\mathbf{w}$, so the equilibrium state $\mathbf{z}$ we just found must be $\mathbf{y}$. Hence $\mathbf{w}$ is within $\kappa C'\mu^{-\frac{1}{2(q\omega-p)}}$ of $\mathbf{y}$. The result follows by using $\xi = 1/\log \mu$ and setting $C'' = \kappa C'$.

□

4 Final remarks

It may be possible to simplify our proof, but the one given is the first we found that works.

Note that shadowing also constructs many other equilibrium states exponentially close to concatenations of discommensurations, given by choosing pseudo-random switch times between long enough segments of discommensuration. This is directly analogous to Palmer’s proof [Pal] of the Birkhoff-Conley-Moser subshift from a transverse homoclinic orbit to a hyperbolic periodic orbit. One can generalise, e.g. allow switching between advancing and retreating discommensurations, provided both have phonon gap.

We expect it is possible to generalise our result to cases where $A_{p/q+}$ is generated by more than one discommensuration, provided they have phonon gap bounded away from zero. If $A_{p/q}$ is also generated by more than one periodic state, however, the exponential bound on the accuracy of approximation will depend in a more complicated way on their coherence lengths.

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