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Physica D 216 (2006) 179–184
PHYSICA D
www.elsevier.com/locate/physd

Discommensuration theory and shadowing in Frenkel–Kontorova models

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Available online 15 March 2006

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

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 discommensurations.

Keywords: Nonlinear physics; Dynamical systems; Frenkel–Kontorova models; Incommensurate structures; Minimum energy states; Discommensurations; Hyperbolicity; Phonon gap; Shadowing theorem

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 [1], Aubry stated that "a configuration with atomic mean distance $l = l_{\text{com}} + \delta l$ ($\delta l > 0$) 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 $l_{\text{com}} = \frac{2ar}{s}$, $2a$ is the period of the potential and r, s are integers). This point of view had also been expressed in [14], where the term "discommensuration" was introduced. It has become very fruitful, e.g. [10,8]. 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 [4], 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 [5], 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 [3], 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 (or 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).

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doi:10.1016/j.physd.2006.01.017

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

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

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 $h : \mathbb{R}^2 \to \mathbb{R}$ is C^2 and satisfies $h(x+1, x'+1) = h(x, x')$ and $h_{12} \le -b$ for some $b > 0$ (subscript i on a function denotes the partial derivative with respect to the ith 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: $W''(\xi) \ge b$. The potential energy of the chain is typically infinite but its gradient and the equilibria are well defined.

Aubry was the first person of whom we are aware to realise that there is a direct connection between a Frenkel–Kontorova model and an associated dynamical system [2]. 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 sizes 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 being 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* [4]). From this and invariance under the *translations* T_{pq},

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

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

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

In fact,

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

where floor(x) is the greatest integer less than x and ceil(x) is the least integer greater than x (this was proved in [12] 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 given in [12]).

Aubry proved there is a minimum energy state for each mean spacing ω [4]. 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 $\mathbf{x} \le \mathbf{y}$ defined by $x_n \le y_n$ 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 $v_n \to L_n$ as $n \to -\infty$, $v_n \to R_n$ as $n \to +\infty$. 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 $n_k \to \infty$ and m_k such that $(x_{n_k} - m_k, x_{n_k+1} - m_k) \to (x_0, x_1)$ as $k \to \infty$). 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 where 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 [13] independently of Aubry), so the subject is often called *Aubry–Mather theory* (for a review, see [9]). 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 a 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 [6].