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Phase-locking in the multidimensional Frenkel-Kontorova model

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We consider the multidimensional Frenkel-Kontorova model with one degree of freedom which is a variational problem for real functions on the lattice $\mathbf{Z}^n$. For every vector $\alpha \in \mathbf{R}^n$ there is a special class of minimal solutions $u_\alpha : \mathbf{Z}^n \to \mathbf{R}$ lying in finite distance to the linear function $x^{n+1} = \alpha x$ with $x \in \mathbf{Z}^n$. Due to periodicity properties of the variational problem α is called the rotation vector of these solutions. The average action $A(\alpha)$ of a minimal solution u_α is obtained by averaging the variational sum over $\mathbf{Z}^n$. One shows that this average action is the same for any minimal solution with finite distance to the linear function $x^{n+1} = \alpha x$ with rotation vector α. Our main results concern the differentiability properties of $A(\alpha)$ as a function of the rotation vector: Typically, A is *not* differentiable at $\alpha \in \mathbf{Q}^n$. This will be interpreted in a dual form as phase-locking. The phase $\alpha(\mu)$ of $\mu \in \mathbf{R}^n$ is defined by the unique vector in $\mathbf{R}^n$ for which $A(\alpha) - \alpha \cdot \mu$ is minimal. If one perturbs the variational principle by changing the parameter μ, the non-differentiability of A at $\alpha \in \mathbf{Q}^n$ forces the phase to be locked onto the rational value $\alpha(\mu)$.

Introduction

The 1-dimensional Frenkel-Kontorova model originates in solid state physics and describes the dislocation of a chain of atoms in a periodic potential with nearest neighbor interactions, see e.g. [2]. Here we consider a generalization where the chain is replaced by a lattice of atoms which have one degree of freedom. One thinks of this degree of freedom as a coordinate describing the dislocations of the atoms in vertical direction (Fig. 1). The steady state positions of the atoms are given by local minima of the Hamiltonian evaluated for each finite set of atoms. This variational problem defines the multidimensional Frenkel-Kontorova model

Mathematics Subject Classification: 70H30, 58C20, 46G05 of one degree of freedom. Configurations which minimize the Hamiltonian on each finite set are called minimal configurations or minimal solutions. To each minimal configuration one assigns the minimal average action which is the mean value of the Hamiltonian per atom. One shows that this minimal average action in fact does only depend on the rotation vector of the minimal configuration. The rotation vector is defined by the average increase in the vertical position of atoms in the i-th direction of the grid.

Given a Hamiltonian depending on some linear and nonlinear parameter we search the rotation vector allowing for an absolute minimum of the minimal average action. This rotation vector at which the minimum is attained is called the phase of the system. It of course depends on the parameters defining the Hamiltonian. Our procedure of finding the phase has two stages: We first fix the rotation vector and look for a corresponding minimal configuration i.e. a configuration which locally minimizes the Hamiltonian and which exhibits the prescribed rotation vector in the large. Then we minimize the average action obtained this way over all rotation vectors and identify the phase as the point where the minimum of the action is reached. We now can ask for the dependency of the phase from the parameters which originally defined the Hamiltonian. As we will show, the phase may be locally constant while the Hamiltonian is tuned by the parameters. We show that the phase typically is locked onto rational rotation vectors while it immediately co-varies (without jump) with the parameters if the components of the phase are rationally independent. The domains in the multidimensional parameter space where phase-locking occur are known as Arnold tongues, cf. Fig. 2. A cut through these tongues at a fixed level of the nonlinear parameter may form an intriguing picture of fractal character as shown in Fig. 3. Considering a single component of the phase as a function of the linear parameter a devil staircase may arise as depicted in Fig. 4.

The phenomenon of phase-locking may be explained by the non-differentiability of the minimal average action at rational rotation vectors. Our main result therefore concerns the differentiability properties of the minimal average action. We show that at rational rotation vectors the minimal average action is typically non-differentiable while is always differentiable at rationally independent rotation vectors. In general, at some rotation vector the minimal average action is always differentiable in directions where there exist no rational dependencies between the components of the rotation vector while it is typically non-differentiable in directions for which rational dependencies exist. In a dual setting the results directly translate to the phase-locking on these rotation vectors for which the minimal average action is not differentiable in any direction. Thus, phase-locking can only occur on rational vectors. In combination with a result of Bangert [6] one knows that for large perturbations of the Hamiltonian such a phase-locking indeed will occur for *any* rational vector in some bounded domain.

The multidimensional Frenkel-Kontorova model with one degree of freedom may be seen as a discrete version of Moser's variational problem on the $(n+1)$-dimensional torus [15] where the discretization restricts to the first n variables. As long as one restricts to the 1-dimensional case, the minimal configurations may be characterized as particular orbits of a twist map of the annulus [14]. Within this setting J. Mather proved differentiability properties of the minimal average action as a function of the rotation number [13]. Such differentiability properties first were investigated by S. Aubry from a physical point of view [2]. V. Bangert obtained the same results from a more geometrical point of view [9]. We generalize these results to a variational problem for real functions on $\mathbf{Z}^n$. The proof of the differentiability properties in case of rational rotation vectors is similar to Mather's one for $n = 1$. In contrast, we deduce the differentiability properties at irrational rotation vectors directly by continuity arguments. We give an explicit formula for the directional derivatives of the minimal average action which in case $n = 1$ is new for irrational rotation numbers. Our proof mainly follows the one given in [19] for the variational problem on the $(n + 1)$-torus.

In Sect. 1 we outline the general model and present the 2-dimensional non-smooth example of F. Vallet[1] [21] as a particular case. His example of an exactly calculable variational problem generalizes Aubry's model in [3]. In Sect. 2 we briefly recapitulate the structure of the set of non-selfintersecting minimal solutions with a given rotation vector. In Sect. 3 we state the differentiability results of the minimal average action as a function of the rotation vector. In Sect. 4 we interpret the non-differentiabilities as phase-locking in the Frenkel-Kontorova model of one degree of freedom. The occurrence of Arnold tongues and devil's staircases will be explained. The proof of the differentiability results is given in Sect. 5.

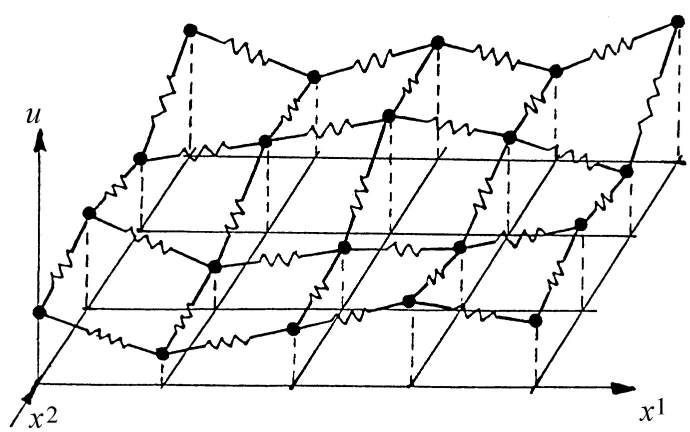

Fig. 1. The particles of the infinite grid are seeking for an equilibrium position between nearest neighbor interactions and the vertical periodic potential. The attractive forces between neighbors are indirectly proportional to their distances. However, the particles are allowed to reduce the distances only by moving in vertical direction.

[1] I would like to thank F. Vallet for the permission to enclose his figures 3 and 4.

1 The multidimensional Frenkel-Kontorova model

We first describe a simple two dimensional model close to Vallet's numerical example. Define the 'Hamiltonian' $H : \mathbf{R}^3 \to \mathbf{R}$ by

$$H(u^0, u^1, u^2) \doteq \frac{c_1}{2}(u^1 - u^0)^2 + \frac{c_2}{2}(u^2 - u^0)^2 + V(u^0) \tag{1}$$

with coupling constants $c_1,\, c_2 > 0$ and a smooth 1-periodic potential $V : \mathbf{R} \to \mathbf{R}$. Given a function $u : \mathbf{Z}^2 \to \mathbf{R}$ describing the dislocation of the particles and some finite set $\Omega \subset \mathbf{Z}^2$ we abbreviate

$$L(u, \Omega) \doteq \sum_{x \in \Omega + \{0, -e_1, -e_2\}} H(u(x), u(x + e_1), u(x + e_2)) \;,$$

where e_1 and e_2 denote the standard basis elements of $\mathbf{Z}^2$. A function $u : \mathbf{Z}^2 \to \mathbf{R}$ is called a **minimal solution** if $L(u + \phi, \Omega) \geq L(u, \Omega)$ for any finitely supported function $\phi : \Omega \to \mathbf{R}$ with $\Omega \subset \mathbf{Z}^2$. For every $\alpha \in \mathbf{R}^2$ there exist minimal solutions $u_\alpha : \mathbf{Z}^2 \to \mathbf{R}$ with $\sup_{x \in \mathbf{Z}^2} |u_\alpha(x) - \alpha x| < \infty$. Since for the i-th component of α one has

$$\alpha^i = \lim_{m \to \infty} \frac{u_\alpha(me_i) - u_\alpha(0)}{m} \;, \quad m \in \mathbf{N} \;,$$

we call α the **rotation vector** of u_α. The **minimal average action** is defined by

$$A(\alpha) \doteq \lim_{r \to \infty} \frac{1}{|\mathbf{Z}^2 \cap B_r|} L(u_\alpha, \mathbf{Z}^2 \cap B_r) \;,$$

where B_r denotes the Euclidean ball in $\mathbf{R}^2$ of radius r and center 0.

If the periodic potential vanishes, $V \equiv 0$, the minimal solutions u_α with $\alpha \in \mathbf{R}^n$ are the affine functions $u_\alpha(x) = \alpha x + c$ on $\mathbf{Z}^2$ with $c \in \mathbf{R}$. The minimal average action in this trivial case is $A(\alpha) = c_1(\alpha^1)^2 + c_2(\alpha^2)^2$. In the example of Vallet [21, Ch. III] the non-smooth potential V in (1) consists of successive parabolic curves with center at the integers $\mathbf{Z}$. It has the form

$$V(u) = \frac{1}{2}(u - [u + \frac{1}{2}])^2 \;,$$

where $[v]$, $v \in \mathbf{R}$, denotes the largest integer $\leq v$.

A generalization of the variational problem to higher dimensions with, however, smooth Hamiltonian is investigated in [10]. In the following we state weaker conditions on the Hamiltonian H which still guarantee existence results for minimal solutions. The conditions are weak enough to include Vallet's example and strong enough to enable to prove the ordering structures for the set of minimal solutions as described in Sect. 2.

The Hamiltonian $H(\mathbb{u})$, $\mathbb{u} = (u^0, \ldots, u^n)$, is assumed to be a continuous function on $\mathbf{R}^{n+1}$ which satisfies

$(H\,1)\quad H(\underline{u}+\underline{1}) = H(\underline{u}) \quad \forall\, \underline{u} \in \mathbf{R}^{n+1}\,,\ \underline{1} = (1,\dots,1)\,,$

$(H\,2)\quad H(\underline{u}) \longrightarrow \infty \ \text{ if } \max_{0\le i,j\le n} |u^i - u^j| \longrightarrow \infty\,,$

$(H\,C^2)\quad H \in C^2(\mathbf{R}^{n+1})$
with $D_iD_jH \le 0$ and $D_iD_0H < 0 \quad \forall\, 1 \le i \ne j \le n$.

In order to include Vallet's non-smooth example we require a generalization of Mather's conditions for $n = 1$ [11, 12]. Let $e_0, e_1, \dots, e_n$ denote the standard unit vectors in $\mathbf{R}^{n+1}$. Instead of $(H\,C^2)$ the following conditions may be imposed:

$(H\,3)\quad H(\underline{u}+\lambda_i e_i + \lambda_j e_j) - H(\underline{u}+\lambda_i e_i) - H(\underline{u}+\lambda_j e_j) + H(\underline{u}) \le 0\,,$
$0 \le i \ne j \le n$. There is $c > 0$ such that for
$1 \le i \ne j \le n\,,\ \lambda_1\,,\ \lambda_i > 0$ and $\underline{u} \in \mathbf{R}^{n+1}$
$H(\underline{u}+\lambda_0 e_0 + \lambda_i e_i) - H(\underline{u}+\lambda_0 e_0) - H(\underline{u}+\lambda_i e_i) + H(\underline{u}) \le -\lambda_0\lambda_i c$.

$(H\,4)$ There is $\theta > 0$ such that for any $\underline{u} \in \mathbf{R}^{n+1}$ and for $\beta = e_0$ or $\beta \in \{0\} \times S^n$ the function $\rho \to \theta\rho^2 - H(\underline{u}+\rho\beta)$ is convex.

Condition $(H\,3)$ states, loosely speaking, that $H(\underline{u})$ is growing if the difference $|u^0 - u^i|$ for some $1 \le i \le n$ is growing. Condition $(H\,4)$ states that H does not have convex corners on the radial lines. Moreover, H is locally Lipschitz in each component u^j, $0 \le j \le n$, by the same reason that this holds for a convex function [17, 10.4].

Put $\mathscr{B} = \{0, -e_1, \dots, -e_n\}$ and let $\Omega + \mathscr{B}$ denote the Minkowski sum of $\mathscr{B}$ and $\Omega \subset \mathbf{Z}^n$. One looks for **minimal solutions** $u : \mathbf{Z}^n \to \mathbf{R}$ which minimize the sum

$$L(u,\Omega) \doteq \sum_{x\in\Omega+\mathscr{B}} H(u(x), u(x+e_1), \dots, u(x+e_n))$$

on every finite set $\Omega \subset \mathbf{Z}^n$ with respect to arbitrary variations of u on Ω. Thus, u is minimal if $L(u+\phi,\Omega) \ge L(u,\Omega)$ for every $\phi : \Omega \to \mathbf{R}$ on every finite set $\Omega \subset \mathbf{Z}^n$. A minimal solution u is said to have **no selfintersection** if the set $\{T_{\overline{k}}u : \overline{k} = (k, k^{n+1}) \in \mathbf{Z}^{n+1}\}$ with $T_{\overline{k}}u(x) \doteq u(x-k) + k^{n+1}$ is totally ordered. A non-selfintersecting minimal solution u exhibits a unique **rotation vector** $\alpha \in \mathbf{R}^n$ with the property $\sup_{x\in\mathbf{Z}^n} |u(x) - \alpha x| < \infty$. By $\mathscr{M}_\alpha$ we denote the set of non-selfintersecting minimal solutions corresponding to α. If $u \in \mathscr{M}_\alpha$ and $x \in \mathbf{Z}^n$ put $\underline{u}(x) \doteq (u(x), u(x+e_1), \dots, u(x+e_n)) \in \mathbf{R}^{n+1}$. As in the 2-dimensional example, the **minimal average action** is defined by

$$A(\alpha) \doteq \lim_{r\to\infty} \frac{L(u, \mathbf{Z}^n \cap B_r)}{|\mathbf{Z}^n \cap B_r|} = \lim_{r\to\infty} \frac{1}{|\mathbf{Z}^n \cap B_r|} \sum_{x\in\mathbf{Z}^n\cap B_r} H(\underline{u}(x))\,,\ u \in \mathscr{M}_\alpha\,,$$

where B_r denotes the ball of radius r and center 0 in $\mathbf{R}^n$. The existence of this limit is not obvious. First one uses that $H(\underline{u}(x))$ is bounded uniformly due to the property $\sup|u(x) - \alpha x| < \infty$ and the Lipschitz continuity of H. Then the existence of the average is shown in the same way as in [18, Lemma 3.3]. Once knowing that the limit exists, it is easy to show that it does not depend on the minimal solution $u \in \mathscr{M}_\alpha$ [18, Lemma 3.2].

2 The set $\mathscr{M}_\alpha$ of non-selfintersecting minimal solutions

A minimal solution $u \in \mathscr{M}_\alpha$ with arbitrary $\alpha \in \mathbf{R}^n$ is said to be **maximally periodic** if $T_{\overline{k}} u = u$ for every $\overline{k} = (k, k^{n+1}) \in \mathbf{Z}^{n+1}$ with $k\alpha = k^{n+1}$. By $\mathscr{M}_\alpha^{per}$ we denote the set of maximally periodic $u \in \mathscr{M}_\alpha$. One shows by a compactness argument that $\mathscr{M}_\alpha \neq \emptyset$ for $\alpha \in \mathbf{Q}^n$. To prove $\mathscr{M}_\alpha \neq \emptyset$ for $\alpha \in \mathbf{R}^n \setminus \mathbf{Q}^n$ one performs a limit process and uses the local Lipschitz continuity of H, compare with the discrete 1-dimensional case [7, (3.3) and (3.17)].

By minimality arguments one shows that $\mathscr{M}_\alpha^{per}$ is **totally ordered**, i.e. for $u, v \in \mathscr{M}_\alpha^{per}$ we have either $u < v$ or $u > v$ or $u \equiv v$, cf. [5]. One may think of the graphs $u \in \mathscr{M}_\alpha^{per}$ as 'leaves' lying in $\mathbf{Z}^n \times \mathbf{R}$. Two cases arise: either the set $\mathscr{M}_\alpha^{per}$ gives rise to a 'foliation' or to a 'lamination' (i.e. 'foliations' with gaps). Motivated from the continuous problem we say that the set $\mathscr{M}_\alpha^{per}$ '**foliates**' $\mathbf{Z}^n \times \mathbf{R}$ if for every $(x, u_\circ) \in \mathbf{Z}^n \times \mathbf{R}$ there exists a unique $u \in \mathscr{M}_\alpha^{per}$ with $u(x) = u_\circ$. $\mathscr{M}_\alpha^{per}$ gives rise to a 'lamination' if there are gaps in the vertical direction such that for some $u_\circ \in \mathbf{R}$ one does not find $u \in \mathscr{M}_\alpha^{per}$ with $u(x) = u_\circ$. For the standard Hamiltonian $H_\circ = \frac{1}{2}\|p\|^2$ the set $\mathscr{M}_\alpha^{per}$ gives to a 'foliation' for any $\alpha \in \mathbf{R}^n$. According to Moser's stability result for the variational problem on the torus [16] one knows that for $\alpha \in \mathbf{Q}^n$ 'not too close to $\mathbf{Q}^n$ ' the 'foliation' survives for small perturbations of $H_\circ$. If, however, the perturbation of $H_\circ$ is large enough the 'foliation' disintegrates, gaps occur and $\mathscr{M}_\alpha^{per}$ gives rise to a 'lamination' for every rationally dependent α in some compact set $K \subset \mathbf{R}^n$. The size of this set K of rotation vectors α for which $\mathscr{M}_\alpha^{per}$ has gaps grows with the size of the perturbation. For Moser's variational principle on the torus this result was proved by Bangert [6]. (Note that in general one only has $\mathscr{M}_\alpha^{per} \supseteq \mathscr{M}_\alpha^{rec}$ where $\mathscr{M}_\alpha^{rec}$ is defined as in [5].)

Let us describe the structure of $\mathscr{M}_\alpha$ if the subset $\mathscr{M}_\alpha^{per}$ has gaps. We say that $\alpha \in \mathbf{R}^n \setminus \mathbf{Q}^n$ is **rationally independent**, if $k\alpha \notin \mathbf{Z}$ for all $k \in \mathbf{Z}^n \setminus \{0\}$. In case that α is rationally independent one knows from the variational problem on the torus that each non-selfintersecting minimal solution $u \in \mathscr{M}_\alpha$ actually is maximally periodic. Thus, $\mathscr{M}_\alpha = \mathscr{M}_\alpha^{per}$ and the set $\mathscr{M}_\alpha$ is totally ordered. The situation is different if α is rationally dependent.

For every $\alpha \in \mathbf{R}^n$ fix some $u_\alpha \in \mathscr{M}_\alpha^{per}$ and put

$$\mathscr{F}_\alpha \doteq \{u(0) : u \in \mathscr{M}_\alpha^{per}\} \cap [u_\alpha(0) - 1, u_\alpha(0)] \,.$$

If $\alpha \in \mathbf{R}^n \setminus \mathbf{Q}^n$ the set $\mathscr{F}_\alpha \subset \mathbf{R}$ has an interesting structure: it is either a closed interval or it contains an infinity of gaps. This is due to the fact that an $u \in \mathscr{M}_\alpha^{per}$ defining a boundary of a gap in $\mathscr{F}_\alpha$ would give rise to an infinity of further gaps in the bounded set $\mathscr{F}_\alpha$ by translating u in directions $\overline{k} \in \mathbf{Z}^{n+1}$ with non-vanishing component k^i for which α^i is irrational. (In case that $\mathscr{M}_\alpha^{per} = \mathscr{M}_\alpha^{rec}$ the set $\mathscr{F}_\alpha$ actually defines a Cantor set, i.e. a closed set of non-isolated points that does not contain an interval (cf. [15, Ch. 6] or [8, (5.5)]). In case that $\mathscr{M}_\alpha$ is a proper supset of $\mathscr{M}_\alpha^{rec}$, however, this does not need to be true anymore.)

Let $\mathscr{G}_\alpha$ be the set of gaps of $\mathscr{F}_\alpha$, i.e. the set of open intervals of $[u_\alpha(0) - 1, u_\alpha(0)] \setminus \mathscr{F}_\alpha$. Suppose that α is rationally dependent and that $\mathscr{M}_\alpha^{per}$ has gaps, i.e. $\mathscr{G}_\alpha \neq \emptyset$. Let us moreover assume that $\alpha^i \in \mathbf{Q}$ for some $1 \leq i \leq n$. For each gap $G = (G^-, G^+) \in \mathscr{G}_\alpha$ we denote by u_G^-, u_G^+, the unique minimal solutions in $\mathscr{M}_\alpha^{per}$ such that $u_G^\pm(0) = G^\pm$. Now, there are further minimal solutions $u_{G,i\pm}$ in $\mathscr{M}_\alpha$ with $u_G^- < u_{G,i\pm} < u_G^+$ and converging to u_G^- and u_G^+ in the directions e_i and $-e_i$, respectively. More precisely the solutions $u_{G,i\pm}$ satisfy

(i) $\quad u_{G,i\pm}(0) \in G$,

(ii) $\quad u_{G,i\pm}$ is maximally periodic up to the direction $\mathbf{Z}e_i$, i.e. for all $\overline{k} \in \mathbf{Z}^{n+1}$ with $\alpha k = k^{n+1}$ and $k^i = 0$ one has $T_{\overline{k}} u_{G,i\pm} = u_{G,i\pm}$,

(iii) $\quad \lim_{m\to\infty} (u_G^+ - u_{G,i\pm})(x \pm me_i) \to 0$ and $\lim_{m\to\infty} (u_{G,i\pm} - u_G^-)(x \mp me_i) \to 0$ uniformly for all $x \in \mathbf{Z}^n$ with $x^i = 0$.

Any minimal solution $u_{G,i\pm}$ satisfying $(i) - (iii)$ is said to be **heteroclinic** in the direction $\pm e_i$. As in the 1-dimensional case the existence e.g. of $u_{G,i+}$ is guaranteed by Aubry's construction taking a sequence of convergent minimal solutions $u_{\tilde{\alpha}} \in \mathscr{M}_{\tilde{\alpha}}^{per}$ with $\tilde{\alpha} \to \alpha$ and $\tilde{\alpha}^i \downarrow \alpha^i$, see e.g. [7, Sect. 5].

Let us define by $\mathscr{M}_{\alpha,i+}^{per}$ the set of maximally periodic solutions together with *all* heteroclinic solutions $u_{G,i+}$ in the direction e_i satisfying $(i) - (iii)$ for some gap G of $\mathscr{M}_\alpha^{per}$. Another possibility to characterize this set is

$$\mathscr{M}_{\alpha,i+}^{per} \doteq \{u \in \mathscr{M}_\alpha \quad : \quad T_{\overline{k}} u = u \text{ for } \overline{k} \in \overline{\Gamma}_{\alpha,i} \text{ and } T_{\overline{k}} u \leq u \text{ for } \overline{k} \in \overline{\Gamma}_\alpha \text{ with } k^i \geq 0\} \; .$$

In case that $\mathscr{M}_\alpha^{per}$ has gaps (and $\alpha^i \in \mathbf{Q}$) the set $\mathscr{M}_{\alpha,i+}^{per}$ is a proper supset of $\mathscr{M}_\alpha^{per}$. Again by minimality arguments one shows that $\mathscr{M}_{\alpha,i+}^{per}$ is totally ordered, cf. [8, (6.13)]. However, by property (iii) (where pairwise the upper and lower signs belong together) the minimal solutions $u_{G,i-}$ and $u_{G,i+}$ 'intersect' and $\mathscr{M}_\alpha$ cannot be totally ordered, cf. [8, (4.8)]. This leads us to the general criterion for the total ordering of $\mathscr{M}_\alpha$:

Lemma 1 *The set $\mathscr{M}_\alpha$, $\alpha \in \mathbf{R}^n$, is totally ordered if and only if the set $\mathscr{M}_\alpha^{per}$ does not have gaps* or *if α is rationally independent.*

Put differently, $\mathscr{M}_\alpha$ is *not* totally ordered if and only if α is rationally dependent *and* $\mathscr{M}_\alpha^{per}$ has gaps.

3 Differentiability properties of the minimal average action

The first two theorems show how the differentiability of $A(\alpha)$ generalizes from the 1- to the multi-dimensional case.

Theorem 1 *A is differentiable at $\alpha \in \mathbf{R}^n$ if and only if the set $\mathscr{M}_\alpha$ of non-selfintersecting minimal solutions with rotation vector α is totally ordered.*

To investigate the case where $\mathscr{M}_\alpha$ is not totally ordered one has to consider the subspace $V_\alpha \doteq \mathrm{span}_{\mathbf{R}}\{k \in \mathbf{Z}^n : \alpha k \in \mathbf{Z}\}$ of directions in which α is rationally dependent. One may think of V_α as the projection to the first n components of the space $\overline{V}_\alpha \doteq \{\overline{k} \in \mathbf{Z}^{n+1} : \overline{\alpha} \cdot \overline{k} = 0\}$ generated by the vectors $\overline{k} \in \mathbf{Z}^{n+1}$ orthogonal to $\overline{\alpha} \doteq (-\alpha, 1)$. Let us denote by $V_\alpha^\perp \subseteq \mathbf{R}^n$ the orthogonal complement of V_α with respect to the standard scalar product in $\mathbf{R}^n$.

Theorem 2 *Suppose $\alpha \in \mathbf{R}^n$, $\beta \in \mathbf{R}^n \setminus \{0\}$ and $\mathscr{M}_\alpha$ is* not *totally ordered. Then A is differentiable at $\alpha \in \mathbf{R}^n$ in the direction β if and only if $\beta \in V_\alpha^\perp$.*

If $\alpha \in \mathbf{R}^n$ with rational first component $\alpha^1 \in \mathbf{Q}$ one could expect that A is differentiable at α in the direction e_1 if there are minimal solutions in $\mathscr{M}_\alpha$ which 'foliate' $\mathbf{Z}^n \times \mathbf{R}$ and which are periodic in the direction e_1. However, this turns out to be not true. The reason is that the existence of the 'foliation' defined by a subset of $\mathscr{M}_\alpha$ does not imply the total ordering of the whole set $\mathscr{M}_\alpha$. If $n \geq 2$ and e.g. $\alpha = (0, 0)$, there may be e_1-periodic solutions in $\mathscr{M}_\alpha$ 'foliating' $\mathbf{Z}^2 \times \mathbf{R}$ and e_1-heteroclinic solutions in $\mathscr{M}_\alpha$ which intersect the periodic ones (cf. [8, Thm. 1] and [19, Fig. 2]).

If $\alpha \in \mathbf{R}^n \setminus \mathbf{Q}^n$ is rationally independent the set $\mathscr{M}_\alpha$ is always totally ordered (Lemma 1) and and A is differentiable at α according to Theorem 1. If $\alpha \in \mathbf{Q}^n$ the set $\mathscr{M}_\alpha$ is *not* totally ordered for generic Hamiltonian H. Hence, A is generically *not* differentiable at $\alpha \in \mathbf{Q}^n$. The situation for $\alpha \in \mathbf{R}^n \setminus \mathbf{Q}^n$ is more subtle. According to the stability result of Moser the 'foliation' disintegrates for large perturbations of $H_\circ = \frac{1}{2}\|p\|^2$ and $\mathscr{M}_\alpha$ is not totally ordered for every rationally dependent α in some compact set $K \subset \mathbf{R}^n$. Assuming such a large perturbation, Theorem 2 states that the (convex) function A restricted to the compact set K exhibits a maximal non-differentiability that a convex function ever can have in a measure theoretic sense: The set of s-singular points of $A|_K$ is the union of countable many compact sets of finite, non-vanishing s-dimensional Hausdorff measure ($s = 0, \ldots, n$), cf. [1, (3.1)]. Recall that α is an **s-singular** point iff A is differentiable at α in at most s linearly independent directions.

The following theorem estimates the difference of right- and left-sided derivative of A in the standard directions e_i. It corresponds to the formula in [13], end of Sect. 3, for the 1-dimensional case.

Theorem 3 *If the i-the component of α is rational and $\alpha^i = \frac{r^i}{s^i}$ with $r^i \in \mathbf{Z}$ and $s^i \in \mathbf{N}$ relatively prime, one estimates*

$$0 \leq (D_{e_i} + D_{-e_i})A(\alpha) \leq const \cdot \frac{1}{s^i} \ ,$$

with some constant depending on H only and some compact set containing α.

Finally we mention that the minimal average action $A(\alpha)$ is *strictly convex*. This is shown in the same way as the strict convexity is shown for the variational principle on the $(n + 1)$-dimensional torus [18].

4 Phase-locking and the dual interpretation

If $V \in C^3(\mathbf{R}/\mathbf{Z})$ is some periodic potential we consider the Hamiltonian

$$H^{\mu,\lambda}(u^\circ, \ldots, u^n) = \frac{c}{2}\|p\|^2 + \lambda V(u^\circ) - \mu p \ , \quad p = (u^1 - u^\circ, \ldots, u^n - u^\circ) \ ,$$

depending on parameter values $\mu \in \mathbf{R}^n$ and $\lambda, c > 0$. The minimal average action corresponding to the Hamiltonian $H^{\mu,\lambda}$ is denoted by $A^{\mu,\lambda}$. Guided from the physical background, the following dual problem arises:

> *Given parameters μ and λ, determine the vector $\alpha = \alpha(\mu, \lambda) \in \mathbf{R}^n$ at which the minimal average action $A^{\mu,\lambda}$ attains its minimum, i.e. such that*
>
> $$A^{\mu,\lambda}(\alpha) = \min_{\tilde\alpha \in \mathbf{R}^n} A^{\mu,\lambda}(\tilde\alpha) \ .$$

Since the function $A^{\mu,\lambda}(\tilde\alpha)$ is convex in $\tilde\alpha$ the minimum exists. Since the function is strictly convex the minimum is attained for exactly one $\tilde\alpha$ and this is denoted by α.

Motivated from the thermodynamical background we call $\alpha = \alpha(\mu, \lambda)$ the **phase** of the system with parameter values μ and λ. One is interested in the phenomenon of **phase-locking**: while the parameters μ and λ vary, the phase $\alpha = \alpha(\mu, \lambda)$ may be locally constant, i.e lock onto some value $\alpha_\circ \in \mathbf{R}^n$. The occurrence of phase-locking is typical for dynamical systems with an underlying periodic structure. The usual way to represent the function $\alpha(\mu, \lambda)$ is to subdivide the parameter space $(\mu, \lambda) \in \mathbf{R}^n \times \mathbf{R}^+$ into regions of constant phase $\alpha_\circ$, i.e. into the subsets $\{(\mu, \lambda) \in \mathbf{R}^n \times \mathbf{R}^+ : \alpha(\mu, \lambda) = \alpha_\circ\}$ with $\alpha_\circ \in \mathbf{R}^n$.

In dynamical systems such a subset of constant phase $\alpha(\mu, \lambda) = \alpha_\circ \in \mathbf{Q}^n$ is known as **Arnold tongue**. Decreasing the parameter λ of the periodic perturbation, $\lambda \downarrow 0$, the intersection of an Arnold tongue with the plane $\mathbf{R}^n \times \{\lambda\}$ gets smaller and smaller until the tongue meets for $\lambda = 0$ the level $\mathbf{R}^n \times \{0\}$ at some point $(\mu_\circ, 0) \in \mathbf{Q}^n \times \{0\}$, see Fig. 2. Since the average action $A^{\mu_\circ,0}$ takes its minimum at $\alpha(\mu_\circ, 0) = \mu_\circ$ we conclude from the condition $\alpha(\mu, \lambda) = \alpha_\circ$ defining a tongue that $\mu_\circ = \alpha_\circ$. Conversely, increasing the parameter $\lambda > 0$, one expects that for any compact set $\Omega \subset \mathbf{R}^n$ the Arnold tongues will fill up the set $\Omega \times \{\lambda_c\}$ at some critical level $\lambda_c > 0$ up to measure zero. Indeed, this theorem was proven by Aubry [4, Thm. 8] for the special case of the 1-dimensional discrete variational problem corresponding to the standard twist map.

We now fix the nonlinearity parameter $\lambda = \lambda_\circ > 0$. The differentiability properties of $A(\alpha)$ then determine the qualitative properties of the function $\alpha(\mu) = \alpha(\mu, \lambda_\circ)$. F. Vallet [21] calculated this function explicitly for the particular 2-dimensional Frenkel-Kontorova model (cf. Sect. 1). Figure 3 shows a cut through the Arnold tongues at level $\mathbf{R}^2 \times \{\lambda_\circ\}$ for different coupling constants. The white convex regions in the (μ_1, μ_2)-plane corresponds to the values where $\alpha(\mu)$ is constant. A cut through the tongue with $\alpha(\mu, \lambda_\circ) = \alpha_\circ$ for some $\alpha_\circ \in \mathbf{Q}^2$ will lead to the set $\mathrm{stab}(\alpha_\circ) \doteq \{\mu \in \mathbf{R}^2 : \alpha(\mu) = \alpha_\circ\}$, one of the white regions in Fig. 3. As we will see, this type of phase-locking calculated by Vallet is typical

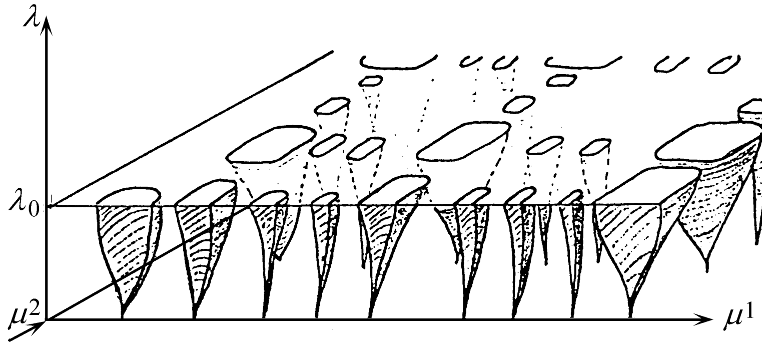

Fig. 2. The Arnold tongues comprising those parameter values $(\mu, \lambda) \in \mathbf{R}^2 \times \mathbf{R}^+$ for which the phase $\alpha(\mu, \lambda)$ takes some fixed value $\alpha_\circ \in \mathbf{R}^2$. A cut through the parameter space at level $\lambda_\circ > 0$ is depicted in Fig. 3.

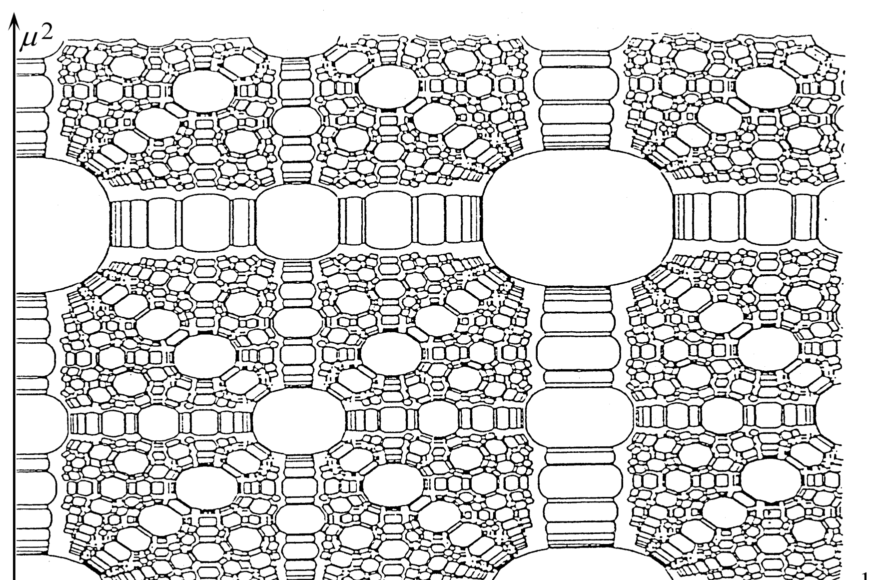

Fig. 3. The collection of subdifferentials $\partial A^0(\alpha)$, $\alpha \in \mathbf{R}^2$, for Vallet's discrete example. For any parameter $\mu = (\mu^1, \mu^2)$ lying within a white convex region $\partial A^\circ(\alpha_\circ)$ (= stab$(\alpha_\circ)$) the phase $\alpha(\mu)$ is locked onto $\alpha_\circ$. (Fig. from [Val].)

for our variational principle. The crucial step is to show that $\mathrm{stab}(\alpha_\circ)$ is the same as the subdifferential $\partial A^0(\alpha_\circ)$. Thereto we need the

Lemma 2 *Let A^μ denote the minimal average action with respect to the Hamiltonian*

$$H^\mu(u^\circ, \dots, u^n) = \frac{c}{2}\|p\|^2 + \lambda_\circ V(u^\circ) - \mu p\ , \quad p = (u^1 - u^\circ, \dots, u^n - u^\circ)\ ,$$

where $V \in C^3(\mathbf{R}/\mathbf{Z})$ and $c,\ \lambda_\circ > 0$. Then, the minimal average action A^μ, $\mu \in \mathbf{R}^n$, and A^0 are related by

$$A^\mu(\tilde\alpha) = A^0(\tilde\alpha) - \mu\tilde\alpha \qquad \forall\ \tilde\alpha \in \mathbf{R}^n\ .$$

Proof. Fix $\tilde\alpha \in \mathbf{R}^n$. For any $\mu \in \mathbf{Z}^n$ let $u^{(\mu)}$ be a minimal solution with respect to H^μ satisfying $\sup_{x\in\mathbf{Z}^n} |u^{(\mu)}(x) - \tilde\alpha x| < \infty$. By the minimality of $u^{(\mu)}$ with respect to H^μ we have

$$\lim_{r\to\infty} \frac{1}{|\mathbf{Z}^n \cap B_r|} L^\mu(u^{(\mu)}, \mathbf{Z}^n \cap B_r) \le \lim_{r\to\infty} \frac{1}{|\mathbf{Z}^n \cap B_r|} L^\mu(u^{(0)}, \mathbf{Z}^n \cap B_r)\ .$$

Using the boundness condition above for $u^{(\mu)}$ with $\mu = 0$ and the regularity of $u^{(0)}$ we obtain $\lim_{r\to\infty} \frac{1}{|\mathbf{Z}^n\cap B_r|} \sum_{x\in\mathbf{Z}^n\cap B_r} p^{(0)}(x) = \tilde\alpha$ where $p^{(0)}(x) = (u^{(0)}(x + e_1) - u^{(0)}(x), \dots, u^{(0)}(x + e_n) - u^{(0)}(x))$. Thus, the right hand side above is equal to

$$\lim_{r\to\infty} \frac{1}{|\mathbf{Z}^n \cap B_r|} L^\mu(u^{(0)}, \mathbf{Z}^n \cap B_r) = \lim_{r\to\infty} \frac{1}{|\mathbf{Z}^n \cap B_r|} L^0(u^{(0)}, \mathbf{Z}^n \cap B_r) - \mu\tilde\alpha\ .$$

Together with the inequality above we obtain the estimate $A^\mu(\tilde\alpha) \le A^0(\tilde\alpha) - \mu\tilde\alpha$. Interchanging the rôle of $u^{(\mu)}$ and $u^{(0)}$ gives the opposite inequality.

□

According to the lemma the phase $\alpha(\mu)$ is defined by

$$A^\mu(\alpha(\mu)) = \min_{\tilde\alpha\in\mathbf{R}^n} A^\mu(\tilde\alpha) = \min_{\tilde\alpha\in\mathbf{R}^n} (A^0(\tilde\alpha) - \mu\tilde\alpha)$$

or, equivalently, by $A^0(\tilde\alpha) \ge A^0(\alpha(\mu)) + \mu \cdot (\tilde\alpha - \alpha(\mu))$ for all $\tilde\alpha \in \mathbf{R}^n$. Therefore, the set $\mathrm{stab}(\alpha_\circ) = \{\mu \in \mathbf{R}^n : \alpha(\mu) = \alpha_\circ\}$ of all parameters μ with the same phase $\alpha_\circ \in \mathbf{R}^n$ is characterized by

$$\mathrm{stab}(\alpha_\circ) = \partial A^0(\alpha_\circ) \doteq \{\mu \in \mathbf{R}^n : A^0(\tilde\alpha) \ge A^0(\alpha_\circ) + \mu \cdot (\tilde\alpha - \alpha_\circ) \ \text{ for all } \tilde\alpha \in \mathbf{R}^n\}\ .$$

The set $\partial A^0(\alpha)$ is called the **subdifferential** of the convex function A^0 at α. If A^0 is differentiable at α, the subdifferential $\partial A^0(\alpha)$ consists of the (sub)gradient $\mu = (D_{e_1} A(\alpha), \dots, D_{e_n} A(\alpha))$ only. The subdifferential is convex since the one-sided directional derivative of a convex function at a given point is itself a convex function of the direction [17, Thm. 23.2]. The diameter of the subdifferential $\partial A^0(\alpha)$ in the direction $\beta \in S^{n-1}$ is given by $(D_\beta + D_{-\beta})A^0(\alpha) \ge 0$.

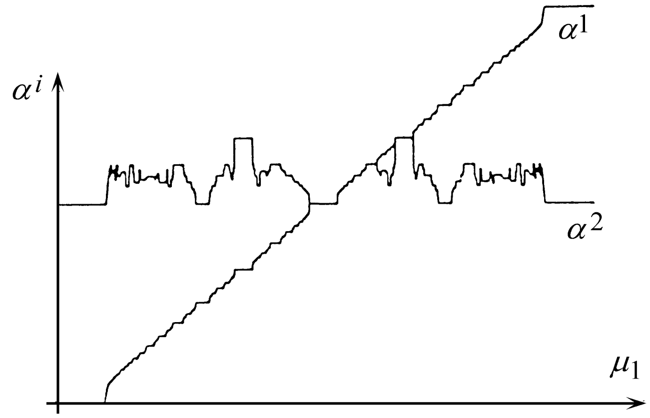

Fig. 4. A plot of the phase functions $\alpha^i(t) \doteq e_i \cdot \alpha(\mu_\circ + te_1)$ for Vallet's example ($i = 1, 2$). The graphs are obtained by varying μ on a horizontal line in Fig. 3. While the first component $\alpha^1(t)$ represents a monotone 1-dimensional devil's staircase, the second component $\alpha^2(t)$ cannot be monotone on a horizontal line. The terrace points of both functions are the same since they correspond to the intersection of the horizontal line with the white convex regions in Fig. 3. (Fig. from [Val].)

Within this dual setting, the phenomenon of **phase-locking** is identified with the existence of nontrivial subdifferentials: if the subdifferential $\partial A^0(\alpha)$ is not just a point, the phase $\alpha(\mu)$ is locked onto $\alpha_\circ$ for all μ varying within the (convex) set $\partial A^0(\alpha)$. By Theorem 2, $\partial A^0(\alpha)$ may contain more than one point only if α is rationally dependent, i.e. if $\alpha k \in \mathbf{Z}$ for some $k \in \mathbf{Z}^n \setminus \{0\}$. Moreover, $\partial A^0(\alpha)$ contains an open ball if and only if $\alpha \in \mathbf{Q}^n$ and $\mathscr{M}_\alpha$ is not totally ordered. As already mentioned the set $\mathscr{M}_\alpha$ is not totally ordered for any α in a given compact set $K \subset \mathbf{R}^n$ if the Hamiltonian is perturbed enough [6]. Assuming this situation, phase-locking will occur at least for any $\alpha \in K \cap \mathbf{Q}^n$.

Finally, let us point out the connection with the popular notion of the 'devil's staircase'. By a n-dimensional **devil's staircase** one may define a continuous, non-constant function $f : \Omega \to \mathbf{R}^n$ on some compact domain $\Omega \subset \mathbf{R}^n$ such that for each rational value $\tilde{\alpha} \in \operatorname{im} f \cap \mathbf{Q}^n$ the pre-image $f^{-1}(\tilde{\alpha})$ is homeomorphic to the unit ball $B_1 = \{\mu \in \mathbf{R}^n : \|\mu\| \le 1\}$. For $n = 1$ this definition corresponds to the usual one of a devil's staircase if one in addition requires monotonicity.

Now, consider the Hamiltonians H^μ, $\mu \in \mathbf{R}^n$, and suppose that for $\mu = 0$ the set $\mathscr{M}_{\tilde{\alpha}}$ is not totally ordered for any $\tilde{\alpha} \in K \doteq [0,1]^n$. Defining $\Omega \doteq \bigcup_{\alpha \in K} \partial A^0(\tilde{\alpha})$ the phase function $\alpha : \Omega \to \mathbf{R}^n$, $\mu \to \alpha(\mu)$, is a n-dimensional devil's staircase. Indeed, for any $\tilde{\alpha} \in K \cap \mathbf{Q}^n$ the subdifferential $\partial A^0(\tilde{\alpha}) = \alpha^{-1}(\tilde{\alpha})$ is homeomorphic to the n-dimensional unit ball B_1^n according to Theorem 2. Moreover, for any point $\mu_\circ \in \Omega$ there is a dense set of directions $\beta \in S^{n-1}$ such that the function $t \longmapsto \beta \cdot \alpha(\mu_\circ + t\beta)$ is a 1-dimensional (not necessarily monotone) devil's staircase. Figure 4 shows the function $t \longmapsto e_1 \alpha(\mu_\circ + te_1)$ for Vallet's numerical example with $n = 2$.

Actually, the family of level sets of $\alpha(\mu)$ has more structure than required by a devil's staircase. Let us assume the situation from above and let $r = r(\tilde{\alpha})$

denote the dimension of $V_{\tilde\alpha} = \mathrm{span}_{\mathbf{R}}\{k \in \mathbf{Z}^n : \tilde\alpha k \in \mathbf{Z}\}$ with $\tilde\alpha \in K$. According to Theorem 2 for every $\tilde\alpha \in K$ the subdifferential $\partial A^0(\tilde\alpha) = \alpha^{-1}(\tilde\alpha)$ at $\tilde\alpha$ is homeomorphic to the r-dimensional unit ball $B_1^r \subset \mathbf{R}^r$. The dual formulation states that $\tilde\alpha$ is a s-singular point of the minimal average action $A^0(\tilde\alpha)$, $s = n - r$.

The boundary structure of $\partial A^0(\tilde\alpha)$ may be investigated iteratively by studying secondary laminations defined by subsets of $\mathscr{M}_{\tilde\alpha}$. For instance, $\partial A^0(\tilde\alpha)$ has a nontrivial $(r-\rho)$-dimensional face if $(D_{\beta_1,\dots,\beta_\rho} + D_{\beta_1,\dots,-\beta_\rho})A^0(\tilde\alpha) > 0$ with linearly independent directions $\beta_i \in V_{\tilde\alpha}$. Now, this last inequality holds if and only if the subset of minimal solutions in $\mathscr{M}_{\tilde\alpha}$ which are 'iteratively heteroclinic' in the directions $\beta_1, \beta_2, \dots, \beta_\rho$, has gaps. For a more precise statement relating the structure of $\partial A^0(\tilde\alpha)$ and $\mathscr{M}_{\tilde\alpha}$ we refer to [20, Ch. 4].

5 Proof of the differentiability properties of $A(\alpha)$

We first state explicit formulas for the directional derivatives of $A(\alpha)$ in the standard unit directions $\pm e_i$, $1 \le i \le n$ (Subsect. 5.1). Our main theorems then may directly be inferred from these formulas (Subsect. 5.2). The proof of the formulas itself is given in Subsect. 5.3.

5.1 The formula for the directional derivatives $D_{\pm e_i}A(\alpha)$

Let $\alpha \in \mathbf{R}^n$ and suppose that the set of gaps $\mathscr{G}_\alpha \neq \emptyset$. For $G \in \mathscr{G}_\alpha$ let $u_G^-, u_G^+ \in \mathscr{M}_\alpha^{per}$ be the 'bottom' and 'top' solution limiting the gap G (cf. Sect. 2). For any $G \in \mathscr{G}_\alpha$ and any subset $\Omega \subseteq \mathbf{Z}^n$ we abbreviate

$$B_G(\Omega) \doteq \sum_{x\in\Omega} H(\underline{u}_G^-(x)) - H(\underline{u}_G^+(x)) \,.$$

Without loss of generality we assume that $\alpha \in \mathbf{R}^n$ is of the form $\alpha = (\alpha^1, \dots, \alpha^r, \alpha^{r+1}, \dots, \alpha^n)$ with $\alpha^1, \dots, \alpha^r \in \mathbf{Q}$ and $\alpha^{r+1}, \dots, \alpha^n \in \mathbf{R}\setminus\mathbf{Q}$ being rationally independent.

A) Case $\alpha^i \in \mathbf{R}\setminus\mathbf{Q}$, i.e. $r+1 \le i \le n$

As we will show the derivatives of A at α in the directions $\pm e_i$ with $\alpha^i \in \mathbf{R}\setminus\mathbf{Q}$ are given by

$$D_{\pm e_i}A(\alpha) = \pm \int_{\mathscr{F}_\alpha} D_i H(\underline{u}(0))\, du^\circ + \sum_{G\in\mathscr{G}_\alpha} B_G(\mathbf{Z}^{\pm} e_i) \tag{2}$$

with $\mathbf{Z}^+ \doteq \{0, 1, 2, \dots\}$ and $\mathbf{Z}^- \doteq \{-1, -2, \dots\}$. The notation makes use of the fact that for every $u^\circ \in \mathscr{F}_\alpha$ there is a unique $u \in \mathscr{M}_\alpha^{per}$ with $u(0) = u^\circ$. By an argument of Mather the partial derivatives D_iH of H at $\underline{u}(0)$ exist due to $(H\,4)$ and the minimality of u, see [13, Sect. 4]. To be precise, the sum in (2) is only defined for α with $\alpha^j = 0$ ($j \neq i$). In this case $\mathbf{Z}e_i$ is a periodicity domain of the solutions in $\mathscr{M}_\alpha^{per}$. In the general case, B_G has to be evaluated on half of a periodicity domain of $u \in \mathscr{M}_\alpha^{per}$ and the sum over $\mathscr{G}_\alpha$ has to be restricted to those gaps G which cannot be transfered into each other by integer translations orthogonal to e_i. Thereto we define $\Gamma_\alpha \doteq \{k \in \mathbf{Z}^n : k\alpha \in \mathbf{Z}\}$ and we let E_α be a fundamental domain of $\mathbf{Z}^n/\Gamma_\alpha$ of the form

$$E_\alpha = \{0, 1, \ldots, s^1 - 1\} \times \cdots \times \{0, 1, \ldots, s^r - 1\} \times \mathbf{Z}^{n-r} \ ,$$

where $\alpha^j = \frac{r^j}{s^j}$ ($1 \leq j \leq r$) with $r^j \in \mathbf{Z}$ and $s^j \in \mathbf{N}$ in lowest terms. If $r^j = 0$ set $s^j = 1$. Note that E_α is a periodicity domain of any $u \in \mathscr{M}_\alpha^{per}$. For $1 \leq i \leq n$ put $E^\circ_{\alpha,i} \doteq \{x \in E_\alpha : k^i = 0\}$, $E^\pm_{\alpha,i} \doteq E^\circ_{\alpha,i} + \mathbf{Z}^\pm e_i$ and $E_{\alpha,i} \doteq E^\circ_{\alpha,i} + \mathbf{Z}e_i$. Let $\mathscr{G}_\alpha/\sim$ be a system of representatives of the equivalence relation $\sim$ on $\mathscr{G}_\alpha$ defined by

$$G_1 \sim G_2 \ :\Longleftrightarrow\ \exists\, \overline{k} \in \mathbf{Z}^{n+1} \text{ with } k^i = 0 \text{ such that } \ G_1 = G_2 - \overline{k} \ .$$

Now, $B_G(E^\pm_{\alpha,i}) = \sum_{G'} B_{G'}(\mathbf{Z}^\pm e_i)$ where the sum is taken over all $G' \in \mathscr{G}_\alpha$ with $G' \sim G$. Formula (2) reduces to

$$D_{\pm e_i}A(\alpha) = \pm \int_{\mathscr{F}_\alpha} D_i H(\underline{u}(0))\, du^\circ + \sum_{G \in \mathscr{G}_\alpha/\sim} B_G(E^\pm_{\alpha,i}) \ . \tag{3}$$

The sum defining $B_G(E^\pm_{\alpha,i})$ exists since $\sum_{x \in E^\pm_{\alpha,i}} u^+_G(x) - u^-_G(x) \leq 1$ by the non-selfintersection property of $u^\pm_G$. Here we use the local Lipschitz-continuity of H. The sum in (3) is absolutely convergent since $\sum_{G \in \mathscr{G}_\alpha/\sim} \sum_{x \in E^\circ_{\alpha,i}} u^+_G(x) - u^-_G(x) \leq 1$ and since by the following Lemma 3 one estimates $|B_G(E^\pm_{\alpha,i})| \leq \text{const} \cdot \sum_{x \in E^\circ_{\alpha,i}} (u^+_G(x) - u^-_G(x))$.

B) Case $\alpha^i \in \mathbf{Q}$, i.e. $1 \leq i \leq r$

In order to state the formula for the derivative in the direction e_i at $\alpha \in \mathbf{R}^n$ with $\alpha^i \in \mathbf{Q}$ we define the subset $\mathscr{M}^{per}_{\alpha\pm} \subseteq \mathscr{M}^{per}_{\alpha,i\pm}$ by

$$\mathscr{M}^{per}_{\alpha\pm} \doteq \mathscr{M}^{per}_\alpha \cup \{T_{\overline{k}} u_{G,i\pm} : G \in \mathscr{G}_\alpha, \overline{k} \in \mathbf{Z}e_i + \mathbf{Z}e_{n+1}\} \ ,$$

where for every gap $G \in \mathscr{G}_\alpha$ we take only *one* heteroclinic solution $u_{G,i\pm}$ satisfying $(i) - (iii)$. Put $\mathscr{F}_{\alpha\pm} \doteq \{u(0) : u \in \mathscr{M}^{per}_{\alpha\pm}\} \cap [u_\alpha(0) - 1, u_\alpha(0)]$ and let $\mathscr{G}_{\alpha\pm}$ denote the set of gaps of $\mathscr{F}_{\alpha\pm}$, i.e. the set of open intervals of $[u_\alpha(0) - 1, u_\alpha(0)] \setminus \mathscr{F}_{\alpha\pm}$. Now, the directional derivatives $D_{\pm e_i}A(\alpha)$ in case $\alpha^i \in \mathbf{Q}$ have the form

$$D_{\pm e_i}A(\alpha) = \pm \int_{\mathscr{F}_\alpha} D_i H(\underline{u}(0))\, du^\circ + \sum_{J \in \mathscr{G}_{\alpha\pm}/\sim} B_J(E^\pm_{\alpha,i}) \tag{4}$$

To prepare the proof of the theorems we rearrange the sum in a more convenient way. Note that every gap $G \in \mathscr{G}_\alpha/\sim$ is - up to boundary points - the disjoint union of gaps $J \in \mathscr{G}_{\alpha\pm}/\sim$. The sum over all these J is a sum of telescope and reduces to

$$B_G^{\pm}(E_{\alpha,i}) \doteq \sum_{J\subset G} B_J(E_{\alpha,i}^{\pm}) = \sum_{x\in E_{\alpha,i}} H(\underline{u}_{G,\pm}(x)) - H(\underline{u}_G^{\pm}(x)) \,, \tag{5}$$

which exists since $u_{G,i+}$ and $u_{G,i-}$ converge (due to the non-selfintersection property quickly enough) to u_G^+ and u_G^- in the directions $\mathbf{Z}^+e_i$ and $\mathbf{Z}^-e_i$, respectively. Formula (4) becomes

$$D_{\pm e_i}A(\alpha) = \pm\int_{\mathscr{T}_\alpha} D_iH(\underline{u}(0))\,du^\circ + \sum_{G\in\mathscr{G}_\alpha/\sim} B_G^{\pm}(E_{\alpha,i}) \;. \tag{6}$$

In case $n = 1$ this variant of (4) corresponds to the formula for $K_I^{\pm}$ in [11, Sect. 3] (where the + in front of the integral has to be replaced by $\pm$).

The following lemma shows how by minimality arguments the sum $B_G(E_{\alpha,i}^{\pm})$ over the domain $E_{\alpha,i}^{\pm} = E_{\alpha,i}^{\circ} + \mathbf{Z}^{\pm}e_i$ may be reduced to a sum over $E_{\alpha,i}^{\circ}$ only.

Lemma 3 *Let $\alpha \in \mathbf{R}^n$ be as above, $1 \le i \le n$. Let the gap $G \in \mathscr{G}_\alpha$ ($G \in \mathscr{G}_{\alpha+}$ in case $1 \le i \le r$, respectively) be of the form $G = (u^-(0), u^+(0))$ with $u^{\pm} \in \mathscr{M}_\alpha^{per}$ ($\mathscr{M}_{\alpha+}^{per}$, respectively). For $\tau \in \mathbf{Z}$ put $E_{\alpha,i}^{\tau} \doteq \{x \in E_{\alpha,i} : x^i = \tau\}$, $E_{\alpha,i}^{\tau+} \doteq \{x \in E_{\alpha,i} : x^i \ge \tau\}$ and $E_{\alpha,i}^{\tau-} \doteq \{x \in E_{\alpha,i} : x^i < \tau\}$. Setting $\triangle_G^{\tau} \doteq \max\{(u^+ - u^-)(x) : x \in E_{\alpha,i}^{\tau}$ or $x \in E_{\alpha,i}^{\tau} + e_i\,,\ 1 \le i \le n\}$ we have*

$$B_G(E_{\alpha,i}^{\tau\pm}) = \pm\sum_{x\in E_{\alpha,i}^{\tau}} (u^+(x) - u^-(x))D_iH(\underline{u}^+(x-e_i)) + O((\triangle_G^{\tau})^2) \;. \tag{7}$$

Proof. Without loss of generality we set $\tau = 0$ and we consider only the version +. We define functions $v^{\pm} : \mathbf{Z}^n \to \mathbf{R}$ by

$$v^+(x) \doteq \begin{cases} u^+(x) & \text{if } x^i \le 0 \\ u^-(x) & \text{if } x^i > 0 \end{cases} \quad , \quad v^-(x) \doteq \begin{cases} u^-(x) & \text{if } x^i \le 0 \\ u^+(x) & \text{if } x^i > 0 \end{cases} \quad .$$

By minimality of $u^{\pm}$ one has $\sum H(\underline{v}^{\pm}(x)) - H(\underline{u}^{\pm}(x)) \ge 0$ where the sum is taken over all $x \in E_{\alpha,i}^+$. Since $v^{\pm}(x) = u^{\mp}(x)$ for $x^i > 0$, the inequalities imply

$$\sum_{x\in E_{\alpha,i}^{\circ}} H(\underline{u}^-(x)) - H(\underline{v}^+(x)) \le B_G(E_{\alpha,i}^+) \le \sum_{x\in E_{\alpha,i}^{\circ}} H(\underline{v}^-(x)) - H(\underline{u}^+(x)) \;.$$

We claim that lower and upper bound may be estimated by an expression differing only of order $O((\triangle_G^{\tau})^2)$. Taking e.g. the lower bound we show

$$\sum_{x\in E_{\alpha,i}^{\circ}} H(\underline{u}^-(x)) - H(\underline{v}^+(x)) =$$

$$-\sum_{x\in E_{\alpha,i}^{\circ}}\sum_{0\le j\le n} (\triangle(x+e_j)D_jH(\underline{u}^+(x)) + O(\triangle(x+e_j)^2)) \,, \tag{8}$$

where $e_\circ \doteq 0$ and $\triangle(x) \doteq u^+(x) - v^-(x) = v^+(x) - u^-(x)$ for $x \in \mathbf{Z}^n$. Note that by the Lipschitz property of H for each component u^i the partial derivatives exist almost everywhere on intervals. For $j = i$ the summation term in (8) vanishes since $\triangle(x + e_i) = 0$ by definition. Due to the periodicities of $u^\pm$ and H one has for $j \neq i$

$$\sum_{x \in E^\circ_{\alpha,i}} \triangle(x + e_j) D_j H(\underline{u}^+(x)) = \sum_{x \in E^\circ_{\alpha,i}} \triangle(x) D_j H(\underline{u}^+(x - e_j)) .$$

Next we use that the discrete Euler equation arising from the condition $\frac{\partial}{\partial u^\circ} L(u^+, x) = 0$ has the form $\sum_{0 \le j \le n} D_j H(\underline{u}^+(x - e_j)) = 0$. Both these facts together reduce the first summation term in (8) to

$$- \sum_{x \in E^\circ_{\alpha,i}} \sum_{0 \le j \le n} \triangle(x + e_j) D_j H(\underline{u}^+(x)) = \sum_{x \in E^\circ_{\alpha,i}} \triangle(x) D_i H(\underline{u}^+(x - e_i)) .$$

The second summation term in (8) is of order $-\sum_{x \in E^\circ_{\alpha,i}} \sum_{0 \le j \le n} O(\triangle(x+e_j)^2) = O((\triangle^\tau_G)^2)$ since $\sum_{x \in E^\tau_{\alpha,i}+e_j} \triangle(x) \le 1$ for any $\tau \in \mathbf{Z}$ and any $0 \le j \le n$. This simplifies (8) to

$$\text{(9)} \quad \sum_{x \in E^\circ_{\alpha,i}} H(\underline{u}^-(x)) - H(\underline{v}^+(x)) = \sum_{x \in E^\circ_{\alpha,i}} \triangle(x) D_i H(\underline{u}^+(x - e_i)) + O(\triangle^2_G) .$$

Since the corresponding equality holds for the upper bound of $B_G(E^+_{\alpha,i})$ the version + of the lemma is proved.

□

5.2 Proof of Theorem 1–3 via formula for $D_{\pm e_i} A(\alpha)$

Proof of Theorem 1 Suppose $\mathscr{M}_\alpha$ is totally ordered and let us assume firstly that the set $\mathscr{M}^{per}_\alpha$ does not have gaps (Lemma 1). By (3) and (4) we trivially have $(D_{e_i} + D_{-e_i}) A(\alpha) = 0$ for $1 \le i \le n$ since $\mathscr{G}_\alpha = \emptyset$. By convexity of A we conclude that A is differentiable at α [17, Thm. 25.2].

Let us assume secondly that $\mathscr{M}^{per}_\alpha$ has gaps and that α is rationally independent. Adding the two versions $\pm$ of (3) we get

$$\begin{aligned} (D_{e_i} + D_{-e_i}) A(\alpha) &= \sum_{G \in \mathscr{G}_\alpha/\sim} B_G(E^+_{\alpha,i}) + B_G(E^-_{\alpha,i}) \\ &= \sum_{G \in \mathscr{G}_\alpha/\sim} B_G(E_{\alpha,i}) = 0 . \end{aligned} \tag{10}$$

The second equality is due to the fact that $E_{\alpha,i}$ is the disjoint union of $E^-_{\alpha,i}$ and $E^+_{\alpha,i}$. To prove the third equality we show that $B_G(E_{\alpha,i}) = 0$ for every $G \in \mathscr{G}_\alpha$. Indeed, $B_G(E_{\alpha,i}) = \lim_{\tau \in \mathbf{Z}^-} B_G(E^{\tau+}_{\alpha,i})$ and by Lemma 3 the term $B_G(E_{\alpha,i})$ converges to 0 for $\tau \to -\infty$ since u^-_G and u^+_G converge asymptotically in the direction $\mathbf{Z}^{-}e_i$. Thus, A is differentiable at α in the directions e_i, $1 \leq i \leq n$. By convexity we again conclude that A is differentiable at α.

Suppose now that $\mathscr{M}_\alpha^{per}$ has gaps and that α is rationally dependent, thus $r \geq 1$. Adding the two versions $\pm$ of (6) we get

$$(D_{e_i} + D_{-e_i})A(\alpha) = \sum_{G \in \mathscr{G}_\alpha/\sim} B_G^+(E_{\alpha,i}) + B_G^+(E_{\alpha,i}) > 0 \ . \tag{11}$$

The reason of the strict inequality is the same as in the 1-dimensional case: Since the solutions $u_{G,i-}$ and $u_{G,i+}$ intersect transversally, their maximum and minimum cannot be minimal due to the 'maximum principle': Since the function u_G^- and u_G^+ are minimal, and since $\max(u_{G,i-}, u_{G,i+})$ and $\min(u_{G,i-}, u_{G,i+})$ converge in the directions $\mathbf{Z}^{\pm}e_i$ asymptotically to u_G^+ and u_G^-, respectively, one gets $B_G^+(E_{\alpha,i}) + B_G^+(E_{\alpha,i}) > 0$. Here, condition ($H$ 3) comes in. The remaining directions $\mathbf{Z}^{\pm}e_j$, $j \neq i$, do not disturb since $u_{G,i-}$ and $u_{G,i+}$ either are periodic or converge asymptotically in these directions. Since (11) establishes the non-differentiability at α, Theorem 1 is proved.

□

Proof of Theorem 2 Suppose $\mathscr{M}_\alpha$ is not totally ordered. According to the Lemma 1 we may assume that α is rationally dependent and that $\mathscr{M}_\alpha^{per}$ has gaps. By convexity of A, the set of directions $\beta \in \mathbf{R}^n \setminus \{0\}$ in which A is differentiable at α is - after adding 0 - a linear subspace of $\mathbf{R}^n$. We therefore restrict to the case that β either lies in $V_\alpha = \text{span}_{\mathbf{R}}\{k \in \mathbf{Z}^n : \alpha k \in \mathbf{Z}\}$ or in $V_\alpha^\perp$. Assuming the special coordinates for α we put $\beta = e_i$ and have $\beta \in V_\alpha$ if $1 \leq i \leq r$, and $\beta \in V_\alpha^\perp$ if $r + 1 \leq i \leq n$. If $\beta \in V_\alpha$ inequality (11) states that A is not differentiable at α in the direction β while in the case $\beta \in V_\alpha^\perp$ equality (10) states that A is differentiable at α in the direction β. This is exactly the statement of Theorem 2.

□

The Proof of Theorem 3 is similar to the one in [19, p. 363] with ω_G^t replaced by $\triangle_G^\tau$.

5.3 Deduction of the formula for $D_{\pm e_i}A(\alpha)$

For $\alpha \in \mathbf{Q}^n$ the formula for the directional derivative generalizes the one obtained in the 1-dimensional case by Mather. We use this formula to deduce by a limit process the formula for irrational rotation vectors $\alpha \in \mathbf{R}^n \setminus \mathbf{Q}^n$. In case $n = 1$ our limit process is simpler than Mather's method since we do not need to estimate the convergence of the difference quotient quantitatively. Mather's argument is replaced by the fact that the corresponding minimal laminations at rational rotation vectors converge to the minimal lamination at the irrational rotation vector.

1) Evaluation of the difference quotient for rational α

By convenience we restrict ourselves to the case $\alpha = 0$. The solutions $u \in \mathscr{M}_\alpha^{per}$ then are constant on $\mathbf{Z}^n$ and formula (6) reduces to

$$D_{\pm e_i} A(0) = \pm \int_{\mathscr{T}_0} D_i H(\underline{u}^\circ)\, du^\circ + \sum_{G \in \mathscr{G}_0} B_G^{\pm}(\mathbf{Z} e_i) \tag{12}$$

with $\underline{u}^\circ = (u^\circ, \ldots, u^\circ) \in \mathbf{R}^{n+1}$ and $B_G^{\pm}(\mathbf{Z}e_i) = \sum_{\nu=-\infty}^{\infty} H(\underline{u}_{G,\pm}(\nu e_i))$. Here we normalized $A(0) = 0$. This formula is exactly the one obtained by Mather in [13, Sect. 3] for the 1-dimensional case. The idea of proof is to write the difference quotient by means of appropriately defined functions w^σ which converge in the limit $\sigma \to \infty$ either to some heteroclinic or periodic $u \in \mathscr{M}_\alpha$. Since w^σ does not need to be minimal, the limit process actually leads only to a relation '$\le$' in (12). To assert the reverse inequality it is possible to estimate the 'angle' $(D_{e_i} + D_{-e_i})A(0)$ of the tangent cone from below by the sum of the right-hand side of (12). Thus, one estimates

$$(D_{e_i} + D_{-e_i})A(0) \ge \sum_{G \in \mathscr{G}_0} B_G^{+}(\mathbf{Z}e_i) + \sum_{G \in \mathscr{G}_0} B_G^{-}(\mathbf{Z}e_i)$$

and concludes that actually the relation '=' in (12) holds. This idea is performed for the variational problem on the torus in [19, Lemma 4 and 5] and is analogous in the present discrete case. For a slight different proof in case $n = 1$ see also [13].

2) Approximation of an irrational α by rational one's

In order to guarantee the formulas (3) and (4) to be true for $\alpha \in \mathbf{R}^n \setminus \mathbf{Q}^n$ we look for a sequence $\tilde\alpha \to \alpha$ with $\tilde\alpha \in \mathbf{Q}^n$ such that left- and right-hand side of (4) with $\tilde\alpha$ in place of α converge separately to the corresponding sides of (3) and (4), respectively. A first condition we impose on the sequence $\tilde\alpha \to \alpha$ is that $\lim_{\tilde\alpha\to\alpha} \frac{\tilde\alpha-\alpha}{\|\tilde\alpha-\alpha\|} = \pm e_i$. By convexity of A this condition implies that the directional derivatives $D_{\pm e_i}A(\tilde\alpha)$ converge to $D_{\pm e_i}A(\alpha)$, cf. [17, Thm. 24.6]. By $B(\alpha, \pm e_i)$ we abbreviate the right-hand side of (3) and (4), respectively, depending on whether α^i is irrational or not. We have to show the convergence $B(\tilde\alpha, \pm e_i) \longrightarrow B(\alpha, \pm e_i)$ for an appropriate sequence $\tilde\alpha \to \alpha$. The idea is that every $u \in \mathscr{M}_\alpha$ occuring in the formula for $B(\alpha, \pm e_i)$ is C^1- approximated on compact sets by functions $\tilde u \in \mathscr{M}_{\tilde\alpha}^{per}$. To guarantee such a C^1- approximation we have to impose additional conditions on the sequence $\tilde\alpha \to \alpha$. If $\alpha' \in \mathbf{R}^n$ put $\overline{\Gamma}_{\alpha'} \doteq \{\overline{k} = (k, k^{n+1}) \in \mathbf{Z}^{n+1} : \alpha' k = k^{n+1}\}$ and $\overline{\Gamma}_{\alpha',i} \doteq \{\overline{k} \in \overline{\Gamma}_{\alpha'} : \overline{k} e_i = 0\}$.

2A) Case $\alpha \in \mathbf{R}^n \setminus \mathbf{Q}^n$ and $\alpha^i \in \mathbf{R} \setminus \mathbf{Q}$

The condition $\overline{\Gamma}_\alpha \subseteq \overline{\Gamma}_{\tilde\alpha}$ ensures that $\tilde u \in \mathscr{M}_{\tilde\alpha}^{per}$ at least has the same periodicity as $u \in \mathscr{M}_\alpha^{per}$. Requiring this condition for every $\tilde\alpha$ implies that each limit of

$\tilde{u} \in \mathscr{M}^{per}_{\tilde{\alpha}}$ with $\tilde{\alpha} \to \alpha$ lies in $\mathscr{M}_\alpha$. Conversely, every $u \in \mathscr{M}^{per}_\alpha$ may be approximated by such $\tilde{u} \in \mathscr{M}^{per}_{\tilde{\alpha}}$ for $\tilde{\alpha} \to \alpha$.

The case that $\mathscr{F}_{\tilde{\alpha}}$ mod **Z** *converges to* $\mathscr{F}_\alpha$ mod **Z** *in measure*
In this case, the proof of $\lim_{\tilde{\alpha}\to\alpha} B(\tilde{\alpha}, \pm e_i) = B(\alpha, \pm e_i)$ splits into two parts corresponding to the summation and integration term in (4) and (3), respectively.

First, if $\tilde{G} \to G$ for $G \in \mathscr{G}_\alpha$ and $\tilde{G} \in \mathscr{G}_{\tilde{\alpha}+}$, one has $\lim_{\tilde{\alpha}\to\alpha} B_{\tilde{G}}(E^+_{\tilde{\alpha},i}) = B_G(E^+_{\alpha,i})$. If otherwise e.g. $\limsup_{\tilde{\alpha}\to\alpha} B_{\tilde{G}}(E^+_{\tilde{\alpha},i}) > B_G(E^+_{\alpha,i})$ then either u^+_G or, for $\tilde{\alpha}$ close to α, $u^-_{\tilde{G}}$ could not be minimal. Here we put $G = (u^-_G(0), u^+_G(0))$ and $\tilde{G} = (u^-_{\tilde{G}}(0), u^+_{\tilde{G}}(0))$ with some appropriate minimal solutions $u^\pm_G$ and $u^\pm_{\tilde{G}}$.

Second, the approximation of the integration term is based on the convergence of $D_i H(\tilde{\text{u}}(0))$ to $D_i H(\text{u}(0))$ for $\tilde{u} \to u$ with $\tilde{u} \in \mathscr{M}^{per}_{\tilde{\alpha}}$ and $u \in \mathscr{M}^{per}_\alpha$. If we do no more claim that H is C^2 this convergence is guaranteed by the convexity condition (H 4): By the same reason that the directional derivatives of a convergent sequence of convex functions are upper semi-continuous [17, Thm. 24.5], the derivatives $D_{\pm e_i} H$ are lower semi-continuous and $\lim_{\tilde{\alpha}\to\alpha} D_{\pm e_i} H(\tilde{\text{u}}(0)) \geq D_{\pm e_i} H(\text{u}(0))$. But according to Mather's minimality argument the partial derivatives $D_i H$ at $\tilde{\text{u}}(0)$ and $\text{u}(0)$ exist and therefore $D_{e_i} H = -D_{-e_i} H \ (= D_i H)$ at these points. This is only possible if in fact $\lim_{\tilde{\alpha}\to\alpha} D_{\pm e_i} H(\tilde{\text{u}}(0)) = D_{\pm e_i} H(\text{u}(0))$.

The case with measure($\mathscr{F}_{\tilde{\alpha}}$) = 0 *while measure*($\mathscr{F}_\alpha$) = 1
This case occurs if $\mathscr{M}^{per}_{\tilde{\alpha}}$ has gaps for every $\tilde{\alpha}$ - as it generically happens for rational rotation vectors - while $\mathscr{M}^{per}_\alpha$ with $\alpha \in \mathbf{R}^n \setminus \mathbf{Q}^n$ 'foliates' $\mathbf{Z}^n \times \mathbf{R}$. The right-hand side of (4) reduces to a pure sum and according to Lemma 3 one has

$$B(\tilde{\alpha}, e_i) = \sum_{\tilde{G}\in\mathscr{G}_{\tilde{\alpha}+}/\sim} B_{\tilde{G}}(E^+_{\tilde{\alpha},i}) = \sum_{\tilde{G}\in\mathscr{G}_{\tilde{\alpha}+}} (u^+_{\tilde{G}}(0) - u^-_{\tilde{G}}(0)) D_i H(\text{u}^+_{\tilde{G}}(-e_i)) + O((\triangle_{\tilde{G}})^2)$$

with $\triangle_{\tilde{G}} \doteq \max_{0\leq j\leq n}(u^+_{\tilde{G}}(e_j) - u^-_{\tilde{G}}(e_j))$. Since the intervals $\tilde{G}$ in $\mathscr{G}_{\tilde{\alpha}+}$ are collapsing for $\tilde{\alpha} \to \alpha$ we get on account of the continuity properties of $D_i H$ deduced above and of Lebesgue's dominated convergence theorem the limit

$$\lim_{\tilde{\alpha}\to\alpha} B(\tilde{\alpha}, e_i) = \int_{\mathscr{F}_\alpha} D_i H(\text{u}(-e_i))\, du^\circ = \int_{\mathscr{F}_\alpha} D_i H(\text{u}(0))\, du^\circ = B(\alpha, e_i)\ .$$

The general case for $\alpha^i \in \mathbf{R} \setminus \mathbf{Q}$
Here, the arguments of the two preceding cases flow in. All one know in general is that $\lim_{\tilde{\alpha}\to\alpha}$ measure($\mathscr{F}_{\tilde{\alpha}}$) $\leq$ measure($\mathscr{F}_\alpha$) for our fixed sequence $\tilde{\alpha} \to \alpha$ satisfying $\overline{\Gamma}_\alpha \subseteq \overline{\Gamma}_{\tilde{\alpha}}$ (and e.g. $\lim_{\tilde{\alpha}\to\alpha} \frac{\tilde{\alpha}-\alpha}{\|\tilde{\alpha}-\alpha\|} = e_i$). For every $\tilde{\alpha}$ let us select the subset $\mathscr{G}^\circ_{\tilde{\alpha}+} \subseteq \mathscr{G}_{\tilde{\alpha}+}$ consisting of those gaps $\tilde{G} \in \mathscr{G}_{\tilde{\alpha}+}$ only which best approximate the gaps $G \in \mathscr{G}_\alpha$. Restricting to this subset we still have

$$\lim_{\tilde{\alpha}\to\alpha} \sum_{\tilde{G}\in\mathscr{G}^\circ_{\tilde{\alpha}+}/\sim} B_{\tilde{G}}(E^+_{\tilde{\alpha},i}) = \sum_{G\in\mathscr{G}_\alpha/\sim} B_G(E^+_{\alpha,i})\ . \tag{13}$$

Since the remaining gaps $\tilde{G} \in \mathscr{G}^1_{\tilde{\alpha}^+} \doteq \mathscr{G}_{\tilde{\alpha}^+} \setminus \mathscr{G}^\circ_{\tilde{\alpha}^+}$ collapse for $\tilde{\alpha} \to \alpha$, the terms $B_{\tilde{G}}(E^+_{\tilde{\alpha},i})$ with $\tilde{G} \in \mathscr{G}^1_{\tilde{\alpha}^+} = \mathscr{G}_{\tilde{\alpha}^+} \setminus \mathscr{G}^\circ_{\tilde{\alpha}^+}$ may contribute in the limit $\tilde{\alpha} \to \alpha$ to the integral term in (3). Taking into account these collapsing gaps one gets with the same technique of Lemma 3

$$(14) \lim_{\tilde{\alpha}\to\alpha} \left(\int_{\mathscr{F}_{\tilde{\alpha}}} D_i H(\underline{u}(0)) du^\circ + \sum_{\tilde{G} \in \mathscr{G}^1_{\tilde{\alpha}^+}/\sim} B_{\tilde{G}}(E^+_{\tilde{\alpha},i}) \right) = \int_{\mathscr{F}_\alpha} D_i H(\underline{u}(0))\, du^\circ \; .$$

Both formulas (13) and (14) together show that for our fixed sequence we have $\lim_{\tilde{\alpha}\to\alpha} B(\tilde{\alpha}, \pm e_i) = B(\alpha, \pm e_i)$ and formula (3) is proved.

2B) Case $\alpha \in \mathbf{R}^n \setminus \mathbf{Q}^n$ and $\alpha^i \in \mathbf{Q}$

In case $\alpha^i \in \mathbf{Q}$ we have to relax the condition $\overline{\Gamma}_\alpha \subseteq \overline{\Gamma}_{\tilde{\alpha}}$ since the solutions $u_{G,i\pm} \in \mathscr{M}^{per}_{\alpha\pm}$ which are not periodic in the directions $\mathbf{Z}^\pm e_i$ have to be approximated as well. We require only that the approximating solutions $u \in \mathscr{M}^{per}_{\tilde{\alpha}}$ have to be periodic with respect to the sublattice of $\overline{\Gamma}_{\tilde{\alpha}}$ with $\overline{k} e_i = 0$. We thus impose the condition $\overline{\Gamma}_{\alpha,i} \subseteq \overline{\Gamma}_{\tilde{\alpha}}$ together with $\tilde{\alpha}^i > \alpha^i$ in case of approximating $\mathscr{M}^{per}_{\alpha^+}$ and $\tilde{\alpha}^i < \alpha^i$ in case of approximating $\mathscr{M}^{mp}_{\alpha-}$. As in 2A) one shows that for the two special assumptions on measure($\mathscr{F}_{\tilde{\alpha}}$) treated there one gets $\lim_{\tilde{\alpha}\to\alpha} B(\tilde{\alpha}, \pm e_i) = B(\alpha, \pm e_i)$.

The general case for $\alpha^i \in \mathbf{Q}$
If $\alpha^i \in \mathbf{Q}$ the inequality $\lim_{\tilde{\alpha}\to\alpha}$ measure($\mathscr{F}_{\tilde{\alpha}}$) $\leq$ measure($\mathscr{F}_\alpha$) needs not to be true anymore. However, it is true if we add to $\mathscr{F}_\alpha$ all points arising from heteroclinic solutions. One shows that $\lim_{\tilde{\alpha}\to\alpha} \mathscr{M}^{per}_{\tilde{\alpha}} = \mathscr{M}^{per}_{\alpha,i+}$ for any sequence $\tilde{\alpha} \to \alpha$ satisfying $\overline{\Gamma}_{\alpha,i} \subseteq \overline{\Gamma}_{\tilde{\alpha}}$ and $\tilde{\alpha}^i > \alpha^i$. (We still assume $\lim_{\tilde{\alpha}\to\alpha} \frac{\tilde{\alpha}-\alpha}{\|\tilde{\alpha}-\alpha\|} = e_i$ to guarantee in addition that $\lim_{\tilde{\alpha}\to\alpha} D_{e_i} A(\tilde{\alpha}) = D_{e_i} A(\alpha)$.) Defining $\mathscr{F}^{all}_{\alpha^+} \doteq \{u(0) : u \in \mathscr{M}^{per}_{\alpha,i+},\, u_\alpha - 1 \leq u \leq u_\alpha\}$ one therefore gets $\lim_{\tilde{\alpha}\to\alpha}$ measure($\mathscr{F}^{all}_{\tilde{\alpha}^+}$) $\leq$ measure($\mathscr{F}^{all}_{\alpha^+}$).

If $\mathscr{G}^{all}_{\alpha^+}$ denotes the gaps of $\mathscr{F}^{all}_{\alpha^+} \subset \mathbf{R}$ we claim that (4, version +) is equivalent to

$$(15) \qquad D_{e_i} A(\alpha) = \int_{\mathscr{F}^{all}_{\alpha^+}} D_i H(\underline{u}(0))\, du^\circ + \sum_{J \in \mathscr{G}^{all}_{\alpha^+}/\sim} B_J(E^+_{\alpha,i}) \; .$$

Since $\mathscr{G}^{all}_{\alpha^+} \subseteq \mathscr{G}_{\alpha^+}$ the sum in (4) in general extends over more gaps J than the sum in (15) and one has to show how an expression $B_J(E^+_{\alpha,i})$ in (4) transforms to a part of the integral in the new formula (15). Let us consider two heteroclinic solutions $u^- < u^+$ in $\mathscr{M}^{per}_{\alpha,i+}$ with $\lim_{m\to\infty}(u^+ - u^-)(me_i) = 0$. Put $J^\pm \doteq u^\pm(0)$ and let us assume that for any $u^\circ \in J \doteq (J^-, J^+)$ there is a further heteroclinic $u \in \mathscr{M}^{per}_{\alpha,i+}$ with $u(0) = u^\circ$, $u^- < u < u^+$. By successive application of Lemma 3 it follows that

$$B_J(E^+_{\alpha,i}) = \int_{J^-}^{J^+} D_i H(\underline{u}(0))\, du^\circ \ .$$

Identifying $B(\tilde{\alpha}, e_i)$ and $B(\alpha, e_i)$ with the right-hand side of (15) (instead of (4+)) for $\tilde{\alpha}$ and α, respectively, the convergence $\lim_{\tilde{\alpha}\to\alpha} B(\tilde{\alpha}, \pm e_i) = B(\alpha, \pm e_i)$ will be proven in exactly the same way as for the case $\alpha^i \in \mathbf{R}\setminus\mathbf{Q}$: Decomposing $\mathscr{G}^{all}_{\tilde{\alpha}+} = \mathscr{G}^{\circ}_{\tilde{\alpha}+} \dot{\cup} \mathscr{G}^{1}_{\tilde{\alpha}+}$ one gets formula (13) with $\mathscr{G}^{all}_{\alpha+}$ in place of $\mathscr{G}_{\alpha}$ and likewise formula (14) with $\mathscr{F}^{all}_{\tilde{\alpha}+}$ and $\mathscr{F}^{all}_{\alpha+}$ in place of $\mathscr{F}_{\tilde{\alpha}}$ and $\mathscr{F}_{\alpha}$, respectively. This shows that $\lim_{\tilde{\alpha}\to\alpha} B(\tilde{\alpha}, \pm e_i) = B(\alpha, \pm e_i)$ in case $\alpha^i \in \mathbf{Q}$ and formula (4) is proved.

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