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EFFECTIVE DISCOMMENSURATIONS IN THE INCOMMENSURATE GROUND STATES OF THE EXTENDED FRENKEL–KONTOROWA MODELS

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For the Frenkel–Kontorowa model and its extensions in several dimensions, with several neighbor interactions, etc., it is proven that the hull function of an incommensurate ground state is purely discrete when the phonon spectrum exhibits a non-zero gap. The same result also holds when the Lyapunov coefficient of the corresponding set of trajectories in the associated twist map (when it is definable) is strictly positive.

When this theorem applies, the Fourier coefficients of the incommensurate modulation can be described by an analytic hull function. This is in some sense a dual result to the Kolmogorov–Arnol’d–Moser theorem, which proves under different hypotheses that incommensurate modulation in real space (instead of reciprocal space) can be described by an analytic hull function.

The physical implication of this theorem is that the incommensurate ground states can be decomposed into a linear superposition of *localized* effective discommensurations. The shape of these discommensurations depends on the model parameters and on their density. Approaching the transition by breaking of analyticity (TBA) from above, the size of these discommensurations diverges. Below the TBA, these discommensurations cannot be described anymore as localized objects in the analytic phase. These results confirm that TBA in non-linear models extends the concept of localization of eigenstates, which up to now was only meaningful for linear operators.

1. Introduction

It has been proven some years ago that the ground states of the Frenkel–Kontorowa (FK) model [1–3] were either commensurate or incommensurate. The commensurate ground states of the FK model are represented in the associated standard map by periodic cycles. The incommensurate ground states may be represented either by Kolmogorov–Arnol’d–Moser (KAM) one-dimensional tori or by Aubry–Mather–Cantor (CAM) sets also called Cantori. In an early preprint [4] (see also ref. [2]), we proposed a theorem (theorem 8) extending the results of theorem 5 in ref. [5], which we did not publish

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later because the proof was lacking in mathematical rigor on some points although the result was exact as we will see here. This theorem asserts that the length of the Cantori representing an incommensurate ground state is zero when the phonon gap of this ground state is non-vanishing. This theorem was quoted and discussed by MacKay et al. in ref. [6]. Modifying our initial proof, they have provided a correct proof for a similar result under a slightly different hypothesis. Instead of requiring a non-zero gap for the phonon spectrum, it is assumed that the Lyapunov coefficient of the trajectory associated with the incommensurate ground state is strictly positive.

Our interest presently returns to this theorem because it appears that it is not only interesting from the mathematical point of view and for the dynamical application to the standard map but also to obtain some rigorous tests of new physical ideas which we are currently developing for coupled electron–phonon systems. For these systems, we also obtained less (but some!) exact results [7] and found that the concept of effective bipolaron should play a role similar to those of effective discommensuration here. Understanding better the electronic behavior in these systems should help both the understanding of charge density waves and of superconductivity. However, these potential physical applications will not be discussed here. They have already been mentioned in ref. [8] (p. 295) and should be discussed with more details elsewhere.

In phenomenological theories [9], it is widely admitted that an incommensurate structure can be described as an array of discommensurations. However, a discommensuration is only well defined when it is unique. When there are many overlapping discommensurations in the same structure, these discommensurations change their shape, energy, etc., but their precise determination becomes ambiguous. We will see here that this theorem on the zero length of the invariant Cantori can give precise informations on this many-body problem. It implies

(1) When the incommensurate ground state is represented by a Cantorus, there is (generally) a unique and unambiguous determination of these discommensurations. It is then obtained as a *linear superposition* of well-defined and localized discommensurations.

(2) The size of the discommensuration diverges at the transition by breaking of analyticity (TBA), that is when the Cantorus becomes a Kolmogorov–Arnol’d–Moser (KAM) torus. When the ground state is represented by a KAM torus, the ground state *cannot be described* by a linear superposition of localized discommensurations.

In this paper, our purpose is to give first a correct proof for this theorem. We do not present now the revised version of the initial proof of ref. [4] but a new proof, which does not use anymore the theory of orthogonal polynomials [2, 4]. Although some of its basic ideas are the same, we have designed this new proof in order that it is not restricted to the one-dimensional nearest-neighbor FK model but apply also to d -dimensional extended FK models. This work has some connection with a recent paper [10] on chaotic trajectories in dynamical systems. Next, we shall describe the physical consequences of this theorem, which allows the exact decomposition of the incommensurate ground states into discommensurations, and give some explicit numerical illustrations.

2. Extended FK models. Summary of early results, the twist map

Let us first describe our notation for the extended FK model [11].^{#1} We consider a d -dimensional square lattice \mathbb{Z}^d where to each site i is associated a scalar atomic displacement u_i . The energy

^{#1}The referee pointed to our attention that this extension of the FK model (with a single atom per unit cell) was recently proposed in this reference [11]. The obtained results are essentially the same as those obtained in ref. [12], although the mathematical language has been reformulated.

functional of this model is

$$\Phi(\{u_i\}) = \sum_{i \in \mathbb{Z}^d, \nu \in \mathbb{B}} L_\nu(u_{i+\nu}, u_i), \quad (1a)$$

where \mathbb{B} is a finite subset of \mathbb{Z}^d which corresponds to the bond directions along which the atoms i and $i + \nu$ interact. Each bond is considered once only, that is if $\nu \in \mathbb{B}$, then $-\nu \notin \mathbb{B}$. For example in models with only nearest-neighbor interaction, \mathbb{B} essentially contains the d basis vectors of \mathbb{Z}^d $(1, 0, \dots, 0)$, $(0, 1, 0, \dots, 0), \dots, (0, 0, \dots, 0, 1)$. But the theory developed here works identically for models with interactions between atoms farther than nearest neighbors providing that this set of bonds \mathbb{B} be finite. For the bond direction ν , the “atoms” i and $i + \nu$ are coupled by potentials $L_\nu(x, y)$. These potentials are chosen with the following properties:

- (1) Functions $L_\nu(x, y)$ are twice differentiable with continuous second-order derivatives.
- (2) Functions $L_\nu(x, y)$ have a lower bound: there exists a constant B , such that for all x, y and ν

$$B \leq L_\nu(x, y). \quad (1b)$$

- (3) Functions $L_\nu(x, y)$ are “diagonally 2π -periodic” that is for all x, y and ν

$$L_\nu(x + 2\pi, y + 2\pi) = L_\nu(x, y). \quad (1c)$$

- (4) There exists a constant C such that for all x, y and ν

$$-\frac{\partial^2 L_\nu(x, y)}{\partial x \partial y} > C > 0. \quad (1d)$$

Extensions of these models where the set of bond directions \mathbb{B} could even be infinite could also be considered. But then we have to modify condition (1d) and to require some extra assumptions in order to get absolute bounds for the interatomic forces. We could also consider models with p -body potentials instead of pair potentials only. We do not consider these possible extensions here. The extrema $\{u_i\}$ of the variational form (1a) satisfy

$$\sum_{\nu \in \mathbb{B}} \frac{\partial L_\nu(u_{i+\nu}, u_i)}{\partial u_i} + \sum_{\nu \in \mathbb{B}} \frac{\partial L_\nu(u_i, u_{i-\nu})}{\partial u_i} = 0. \quad (2a)$$

For this model in one dimension ($d = 1$) with nearest-neighbor interactions, the set \mathbb{B} consists of a single bond so that the index ν can be dropped. It is associated with a twist map [1–3]. Then, this equation becomes

$$\frac{\partial L(u_{n+1}, u_n)}{\partial u_n} + \frac{\partial L(u_n, u_{n-1})}{\partial u_n} = 0, \quad (2b)$$

which by setting

$$p_n = \frac{\partial L(u_n, u_{n-1})}{\partial u_n} \quad (3a)$$

defines the associated twist map T

$$(u_{n+1}, p_{n+1}) = T(u_n, p_n), \quad (3b)$$

which maps a certain domain of the cylinder $\mathbb{C} \times \mathbb{R} = \{u \bmod 2\pi, p\}$ onto itself (see refs. [1–3] for details) by the implicit equations

$$\frac{\partial L(u_{n+1}, u_n)}{\partial u_n} = -p_n \quad (3c)$$

and

$$p_{n+1} = \frac{\partial L(u_{n+1}, u_n)}{\partial u_{n+1}}. \quad (3d)$$

The special case

$$L(x, y) = \frac{1}{2}C(x - y)^2 + \lambda(1 - \cos y) \quad (4a)$$

yields the standard FK model which is associated with the particular twist map called standard map:

$$p_{i+1} = p_i + k \sin u_i, \quad (4b)$$

$$u_{i+1} = u_i + p_i + k \sin u_i \pmod{2\pi}, \quad (4c)$$

$$k = \lambda/C. \quad (4d)$$

For any value of k , it has been proven [1–3] that the incommensurate ground states of models (1a) in one dimension ($d = 1$) can be written as

$$u_i = il + \alpha + g(il + \alpha) = f(il + \alpha) \quad (5a)$$

where α is an arbitrary phase, $\zeta = l/2\pi$ is an irrational number which is the rotation number of the corresponding trajectory $\{u_i, p_i\}$ in the associated twist map. $f(x)$ is a strictly increasing function which is either continuous or can be chosen arbitrarily either left continuous or right continuous when it is discontinuous. (This function $f_\zeta(x)$ also depends on the irrational number ζ .) The modulation hull function $g(x) = f(x) - x$ is 2π -periodic. When $\zeta = l/2\pi = r/s$ is a rational number (with r/s irreducible), the corresponding ground state configuration is commensurate and fulfills for all i : $u_{i+s} = u_i + 2r\pi$.

The same results can be readily extended to the d -dimensional model (1) in the extended form (1) (see refs. [1–3, 12, 13]). Then, for any vector $l = \{l_\mu\} \in \mathbb{R}^d$ ($\mu = 1, 2, 3, \dots, d$) the components l_μ of which are not rationally related, that is for any non-vanishing set of integers $\{p_\mu\} \in \mathbb{Z}^d$ and $p \in \mathbb{Z}$, we have the inequality

$$\sum_{\mu=1}^d p_\mu l_\mu \neq 2p\pi. \quad (5b)$$

There exists an incommensurate ground state described by a hull function (5a) where $il = \sum_{\mu=1}^d i_\mu l_\mu$

denotes a scalar product and α is an arbitrary phase. The hull function $f(x)$ has the same properties as mentioned above for $d = 1$. In particular, $f(x)$ depends on the vector $\zeta = l/2\pi$.

Numerical calculations [12, 13] confirmed that there exists a transition by breaking of analyticity (TBA) in d -dimensional systems as well as in 1D systems. Close enough to the integrable limit $f(x)$ is found to be a smooth function while in the opposite regime close to the anti-integrable [10] limit $f(x)$ is clearly discontinuous.

Results similar to (5a) as well as the results presented in the following can be extended to an even wider class of models with several atomic variables per unit cell. Then, the single variable u_i becomes $u_{i,\iota}$, where ι denotes the atomic variable in the unit cell $i \in \mathbb{Z}^d$. (The number of atoms ι in the unit cell is of course finite.) We also require that all the interaction potentials $L_{\nu}^{\iota,\iota'}(x, y)$ between atom ι in unit cell i and atom ι' in unit cell $i + \nu$ keep the same properties (1b), (1c), (1d) as in the initial model. The result which generalizes (5a) is that for any given $\zeta = l/2\pi$, there exists a set of hull functions $f_{\iota}(x)$ with the same properties as $f(x)$ in (5a) (now there is a different hull function for each kind of atom ι in the unit cell) such that the whole configuration is described by $u_{i,\iota} = f_{\iota}(il + \alpha)$. Functions $f_{\iota}(x) - x$ are 2π -periodic, which implies that the rotation numbers $l = \{l_{\mu}\}$ are the same for each set of variables labelled by ι .

These extended results were already applied some years ago for performing the exact calculation of the phase diagrams of models with piecewise parabolic potentials in two-dimensional models [12, 13] and in one-dimensional models with two atoms per unit [14] cell describing incommensurate structures in an electric field. The results exhibited extended complete Devil’s staircase $l(\mu): \mathbb{R}^2 \rightarrow \mathbb{R}^2$.

We briefly recall the outline of the proof of this theorem. The reader should refer for details to refs. [1–3] and especially ref. [3], where these proofs were simplified. They are practically the same as for the nearest-neighbor one-dimensional case and thus it should not require an extra publication. (These proofs were described in great details in the Ph.D. dissertation of ref. [12] with applications. They also have been published later and independently in ref. [11].

(1) For $\zeta_r = l/2\pi = \{r_{\mu}/s_{\mu}\}$ with irreducible rational components r_{μ}/s_{μ} , commensurate ground states can be constructed. They fulfill for all i, ι and μ , the periodic conditions $u_{i+s_{\mu}|\mu\rangle,\iota} = u_{i,\iota} + 2r_{\mu}\pi$, where $|\mu\rangle$ are the d unit vectors $(1, 0, \dots, 0), (0, 1, 0, \dots, 0), \dots, (0, 0, \dots, 0, 1)$ in the d directions μ of \mathbb{R}^d . Because of condition (1d), a proof similar to those of the fundamental lemma in 1D allows one to prove that for a given rational $\zeta_r = l/2\pi = \{r_{\mu}/s_{\mu}\}$, these ground states are also ground states for the infinite system and that the corresponding set of commensurate ground states is a totally ordered set \mathcal{S}_{ζ_r} .

(2) Using (1c), this set \mathcal{S}_{ζ_r} is globally invariant under the action of an Abelian group G with the $d + 1$ generators g_0 and g_{μ} for $\mu = 1, \dots, d$ defined as

$$g_0(\{u_{i,\iota}\}) = \{u_{i,\iota} + 2\pi\}, \quad \text{and} \quad g_{\mu}(\{u_{i,\iota}\}) = \{u_{i+|\mu\rangle,\iota}\}.$$

Then similarly to the 1D case, for $\zeta = l/2\pi$ with arbitrary irrational components, we can construct a totally ordered continuous family of incommensurate ground states \mathcal{S}_{ζ} as limits of sets of *totally ordered* commensurate ground states \mathcal{S}_{ζ_r} with $\zeta_r \rightarrow \zeta$. Because this set \mathcal{S}_{ζ_r} is also globally invariant under the action of the Abelian group G , the same proof as in refs. [1–3] shows that it is described by a set of hull functions $f_{\iota}(x)$ with the above mentioned properties.

However, it is not possible to prove the reciprocal results, that is all the ground states of model (1) can be obtained by this construction. The simple reason is that this result is generally wrong (except for the nearest-neighbor interaction one-dimensional models considered in refs. [1–3]!). Indeed, it is clear that a much wider variety of boundary conditions can be applied in models with two dimensions and more. Particularly, by forcing non-periodic boundary conditions for finite systems (although they are generally

unphysical), one can obtain in the limit of an infinite system, many kinds of non-periodic and non-quasi-periodic ground states (or minimum energy configurations), where for example the “generalized rotation vector” $\zeta = l/2\pi$ may be undefined. We now close this remark and from now on, we return for sake of simplicity to the model (1) with one atom per unit cell.

According to ref. [10], the quadratic expanded action matrix (QEAM) of a configuration $\{u_n\}$ is the matrix $\mathbf{M} = \{M_{i,j}\}$ of the second variation of the action defined as

$$M_{i,j} = \frac{\partial^2 \Phi(\{u_n\})}{\partial u_i \partial u_j}. \tag{6}$$

For an incommensurate ground state $\{u_i(\alpha)\}$ given by (5a), it is clearly a function $\mathbf{M}(x)$ of its phase $x = \alpha$. In the case of the twist map (1a) ($d = 1$), this matrix is tridiagonal and we have

$$M_{i,j} = 0 \quad \text{for } |i - j| > 1, \tag{7a}$$

$$M_{i,i+1} = \frac{\partial^2 L(u_i + 1, u_i)}{\partial u_i \partial u_{i+1}}, \tag{7b}$$

$$M_{i,i} = \frac{\partial^2 L(u_{i+1}, u_i)}{\partial u_i^2} + \frac{\partial^2 L(u_i, u_{i-1})}{\partial u_i^2}. \tag{7c}$$

Since the ground state configurations are stable configurations, they have the property that their QEAM is positive or zero. In other words, we have for the quadratic form

$$\sum_{i,j} X_i^* M_{i,j} X_j = \langle X | \mathbf{M} | X \rangle \geq 0 \tag{8a}$$

for any vector $X = \{X_i\}$.

Then, it is easy to prove that we have the equivalent definition for $\|\mathbf{M}\|$

$$\|\mathbf{M}\| = \sup_{X \neq 0} \frac{\langle X | \mathbf{M} | X \rangle}{\langle X | X \rangle} \tag{8b}$$

is the supremum of the spectrum of \mathbf{M} and

$$\frac{1}{\|\mathbf{M}^{-1}\|} = \inf_{X \neq 0} \frac{\langle X | \mathbf{M} | X \rangle}{\langle X | X \rangle} \tag{8c}$$

is the infimum of the spectrum of \mathbf{M} . The gap parameter is defined as in ref. [10]:

$$\Delta = \frac{1}{\|\mathbf{M}\| \|\mathbf{M}^{-1}\|}. \tag{9a}$$

When \mathbf{M} is not invertible, Δ is set to be zero. Since by definition, a value z belongs to the spectrum of \mathbf{M} if and only if the inverse operator $(z\mathbf{I} - \mathbf{M})^{-1}$ is defined (with a finite norm), a non-vanishing gap parameter is equivalent to say that zero does not belong to the spectrum of \mathbf{M} . It is clear from the

spectral norm definitions of $\| \cdot \|$, that we have

$$0 \leq \Delta < 1. \tag{9b}$$

3. The discreteness theorem (extended form)

We have proven in the early reference [3]

Theorem 1. For $k > 2\sqrt{\pi^2 + 1}$, the hull function $f(x)$ of any incommensurate ground state of the standard FK model (4) is purely discrete.

As we already pointed out in section 1, we extended this result to ground states with strictly positive gap parameter [4]. With a similar proof, MacKay et al. extended this result [6] with a condition of positivity on the Lyapunov coefficient and Goroff [15] related this result to the uniform hyperbolicity of the set of all ground states. In addition, the Hausdorff dimension of the invariant Cantori was pointed out to be zero under some conditions [16, 17].

A more general version of these theorems can be given for the extended model (1) in any dimension d . The incommensurate ground state $\{u_n\}$ with $u_n = f(nl + \alpha)$ has a monotone increasing hull function $f(x)$ which is either left continuous or right continuous or both with $f(x) - x$ 2π -periodic. The stationary equation (2a) readily yields the functional equation for $f(x)$:

$$\sum_{\nu \in \mathbb{B}} \partial_2 L_\nu(f(x + l_\nu), f(x)) + \sum_{\nu \in \mathbb{B}} \partial_1 L_\nu(f(x), f(x - l_\nu)) = 0, \tag{10a}$$

where we denote by ∂_1 and ∂_2 , the derivation operators with respect to the first and second variable respectively:

$$\partial_2 L_\nu(x, y) = \frac{\partial L_\nu(x, y)}{\partial y}, \quad \partial_1 L_\nu(x, y) = \frac{\partial L_\nu(x, y)}{\partial x}. \tag{10b}$$

In addition, since $\{u_n\}$ is a ground state, the QEAM $\mathbf{M}(\alpha)$ of $\{u_n\}$ is always positive or zero. According to a theorem of Lebesgue [18], any monotone increasing function $f(x)$ can be uniquely decomposed (up to a constant) into the sum of three monotone increasing functions:

$$f(x) = f_{ac}(x) + f_{sc}(x) + f_d(x), \tag{11}$$

where the component $f_{ac}(x)$ is absolutely continuous. This property means that $f_{ac}(x)$ is differentiable almost everywhere with derivative $f'_{ac}(x)$ (i.e. on a set with full Lebesgue measure) and moreover that the variation $f_{ac}(b) - f_{ac}(a)$ of $f_{ac}(x)$ on any interval $[a, b]$ is just equal to $\int_a^b f'_{ac}(x) dx$.

The component $f_{sc}(x)$ is singular continuous. This property means that $f_{sc}(x)$ is continuous but the derivative $f'_{sc}(x)$ is zero for almost all x (that is for a set of x which has full Lebesgue measure). Clearly, the variation of $f_{sc}(x)$ cannot be obtained from its derivative.

The component $f_d(x)$ is discrete, which means that it can be written as a convergent series of jump functions $Y(x)$, i.e. the positive measure $df_d(x)$ is a countable series of Dirac measures $\sum_i f_i \delta(x - x_i)$ with positive amplitudes f_i and locations x_i . This function only varies by discontinuities.

We can associate to any monotone increasing function $f(x)$, a measure $df(x)$ called the Stieltjes measure [19] associated with $f(x)$ which by definition fulfills $\int_a^b df(x) = f(b) - f(a)$ for any couple of points (a, b) where $f(x)$ is not discontinuous.

When the gap parameter Δ of the incommensurate ground state is strictly positive, we obtain theorem 2 which extends theorem 1:

Theorem 2. The hull function $f(x)$ of any incommensurate ground state of model (1) is purely discrete when its gap parameter Δ is strictly non-zero.

The physical consequences of this theorem will be discussed in the next section. We propose now the following conjecture.

Conjecture. When the gap parameter of an incommensurate ground state is zero, the Stieltjes measure $df(x)$ associated with its hull function $f(x)$ is either purely absolutely continuous or purely singular continuous.

Of course, we know that when the associated trajectory in the twist map is a KAM torus, $f(x)$ is an analytic function and thus is purely absolutely continuous. At the TBA, numerical observations of scaling properties suggest [20] that $f(x)$ could be singular continuous. In the non-analytic phase, beyond the TBA, the phonon gap is finite and thus theorem 2 proves that $f(x)$ is purely discrete.

We describe in the main text only the outlines of the proof of theorem 2 while the technical details are left for the appendices: (1) First, we prove (see appendix A)

Proposition 1. The spectrum of the QEAM of $\{u_n(\alpha)\} = \{f(nl + \alpha)\}$ does not depend on the phase α .

Consequently, the gap parameter does not depend on the phase of the incommensurate ground state. Let us note that the proof of this proposition only depends on the property of “weak periodicity” of the ground states (defined in ref. [21]), which is a weaker property than the property of quasi-periodicity. Up to any given accuracy, any local configuration of the ground state with phase α is found again in the same configuration at a bounded distance and also in any other ground state with the same incommensurability ratio ζ and with phase α' .

(2) Next, we prove that the existence of a continuous part in the hull function $f(x)$ of the incommensurate ground state allows one to construct for many phases α , a positive solution $h_n(\alpha)$ to the eigen-equation at zero eigenvalue of the QEAM $\mathbf{M} = \{M_{i,j}\}$ of $\{u_n(\alpha)\}$. More precisely we prove in appendix B the following result:

Proposition 2. Let us assume that the Stieltjes measure $df_c(x)$ (associated with the continuous part $f_c(x)$ of the hull function $f(x)$ of the incommensurate ground states, is not vanishing. Then for any $i \in \mathbb{Z}^d$

(a) the 2π -periodic function

$$h_i(x) = \frac{df_c(x + il)}{df_c(x)}$$

is defined and strictly positive for $x \in \mathcal{A}_i$, where \mathcal{A}_i is a measurable subset of \mathbb{R} which has full measure

with respect to the measure $df_c(x)$. Defining $\mathcal{A} = \bigcap_{i \in \mathbb{Z}^d} \mathcal{A}_i$, we have

$$\int_{x \in \mathcal{A} \cap [0, 2\pi]} df_c(x) = \int_0^{2\pi} df_c(x); \tag{12a}$$

(b) for $x \in \mathcal{A}$, $h_i(x)$ is a strictly positive solution of the eigen-equation of the QEAM for a zero eigenvalue:

$$\sum_j M_{i,j}(x) h_j(x) = 0 \quad \text{for all } i; \tag{12b}$$

(c) for any $i \in \mathbb{Z}^d$, the integral

$$\int_0^{2\pi} h_i(x) df_c(x) = \int_0^{2\pi} df_c(x) \tag{12c}$$

does not depend on i .

This solution $h_n(\alpha)$ is not necessarily bounded for $|n| \rightarrow \infty$ and thus is not necessarily either an eigenvector or a pseudo eigenvector of the QEAM. However, this proposition asserts that the solution $h_n(\alpha)$ integrated over the phase with respect to the measure $df_c(x)$ determined by the continuous part of $f(x)$ does not depend on n . This property is essential for proving that this positive solution cannot grow at infinity “faster than any given exponential” (if it grows). Before proving this result, we prove in appendix C that the existence of a finite gap parameter implies an exponential growth of any positive solution:

Proposition 3. Let us assume that zero does not belong to the spectrum of the QEAM \mathbf{M} and that Ψ_j is an (unbounded) solution with $\Psi_0 = 1$ which fulfills the eigen-equation of an Hermitian matrix \mathbf{M} with zero eigenvalue

$$\sum_j M_{i,j} \Psi_j = 0.$$

Then there exist two positive numbers K and γ where γ only depends on the gap parameter of \mathbf{M} such that for all $n > 0$

$$A_n = \sum_{i \in \mathbb{D}_n} |\Psi_i|^2 > K \exp(\gamma n)$$

where \mathbb{D}_n is defined by the set of sites $i \in \mathbb{Z}^d$ with $\sup_v |i_v| = n$. (This set contains $(2n + 1)^d - (2n - 1)^d$ sites.)

We now define the function

$$H_n(x) = \frac{1}{(2n + 1)^d - (2n - 1)^d} \sum_{i \in \mathbb{D}_n} h_i(x) \tag{13a}$$

for each $n > 0$. Thus, using (12c), it follows that

$$\int_0^{2\pi} H_n(x) df_c(x) = \int_0^{2\pi} df_c(x) \tag{13b}$$

is non-zero and does not depend on n . Using proposition 3, and the inequality

$$\sqrt{\sum_{i \in \mathbb{D}_n} |\Psi_i|^2} \leq \sum_{i \in \mathbb{D}_n} |\Psi_i| \tag{14a}$$

the function

$$K(x) = \inf_{n>0} [(2n + 1)^d - (2n - 1)^d] H_n(x) \exp[-\frac{1}{2}\gamma(\Delta)n] \tag{14b}$$

never vanishes, since because of proposition 1, γ only depends on Δ and is independent of x . Since $K(x)$ is defined as the lower bound of a countable family of measurable functions, it is measurable and we have the strict inequality

$$\int_0^{2\pi} K(x) df_c(x) > 0. \tag{15a}$$

Therefore, we find that

$$\int_0^{2\pi} H_n(x) df_c(x) \geq \exp(\frac{1}{2}\gamma n) \frac{1}{(2n + 1)^d - (2n - 1)^d} \int_0^{2\pi} K(x) df_c(x) \tag{15b}$$

should diverge exponentially for $n \rightarrow \infty$ and thus cannot be a constant. The existence of a non-constant continuous part in $f(x)$ is incompatible with a non-zero gap parameter Δ . Thus, theorem 2 is proven.

In the particular case of the twist map (model with nearest-neighbor interaction in one dimension), the assumption that the Lyapunov coefficient of the trajectory in the twist map associated with the incommensurate ground state $\{u_n(\alpha)\}$ is strictly positive, can be used instead of proposition 3. As we pointed in ref. [10], the Lyapunov coefficient of a trajectory may be non-zero while the gap parameter vanishes. However, we believe that for the ground state trajectories, there is an equivalence between a vanishing gap parameter and a vanishing Lyapunov coefficient. Since we did not prove this result, let us show that we can recover nevertheless the result proposed by MacKay et al. [6].

Theorem 2'. For the nearest-neighbor one-dimensional FK model associated with a twist map by eqs. (3), the hull function of the incommensurate ground state is purely discrete when the Lyapunov coefficients of the associated trajectories in the twist map are strictly positive and larger than some number $\kappa > 0$.

To prove this result, we note that we have from the definition of $h_n(x)$

$$h_n(x) = \frac{df_c(x + nl)}{df_c(x)} = \frac{1}{h_{-n}(x - nl)}. \tag{16a}$$

Then, it follows that

$$\int_0^{2\pi} h_n(x) df_c(x) = \int_0^{2\pi} \frac{1}{h_n(x)} df_c(x) = \text{constant}. \quad (16b)$$

Let us now consider $\kappa > 0$, a strict lower bound for the Lyapunov coefficient of $\{u_n(\alpha)\}$ for all phases α (although it probably does not depend on the phase α). When the gap parameter is non-vanishing, this assertion can be proven by using the Thouless formula and by noting that the momenta of the density of states are phase independent. These arguments are closely similar to those developed for a different problem in ref. [5], section 4.4). We define two 2π -periodic positive measurable functions $H_1(x)$ and $H_2(x)$ by

$$H_1(x) = \inf_n h_n(x) \exp(-\kappa|n|) \quad (17a)$$

and

$$H_2(x) = \inf_n \frac{1}{h_n(x)} \exp(-\kappa|n|), \quad (17b)$$

which yields

$$I_n = \int_0^{2\pi} h_n(x) df_c(x) \geq \exp(\kappa|n|) \int_0^{2\pi} H_1(x) df_c(x) \geq 0 \quad (18a)$$

and

$$I_n = \int_0^{2\pi} \frac{1}{h_n(x)} df_c(x) \geq \exp(\kappa|n|) \int_0^{2\pi} H_2(x) df_c(x) \geq 0. \quad (18b)$$

Since I_n must be independent of n , it follows that

$$\int_0^{2\pi} H_1(x) df_c(x) = 0 \quad (19a)$$

and

$$\int_0^{2\pi} H_2(x) df_c(x) = 0. \quad (19b)$$

Then, we must have $H_1(x) = 0$ and $H_2(x) = 0$, for almost all x with respect to the measure $df_c(x)$. This result means

$$\liminf_{n \rightarrow \pm\infty} h_n(x) \exp(-\kappa|n|) = 0 \quad (20a)$$

and

$$\liminf_{n \rightarrow \pm\infty} \frac{1}{h_n(x)} \exp(-\kappa|n|) = 0. \quad (20b)$$

Since we assume that the Lyapunov coefficient of the incommensurate ground states is defined for all phases and is strictly positive, $h_n(x)$ either diverges exponentially or converges exponentially to zero with a coefficient strictly larger than κ . Conditions (20) cannot be both fulfilled, which proves that theorem 2 is also valid when the Lyapunov coefficient is supposed to be strictly positive instead of the gap parameter.

4. Discontinuity classes

When the gap parameter Δ of an incommensurate ground state of the FK model [1-3] or of its extension (1a) is strictly positive, it is now proven that $f(x)$ is a discrete function and thus is discontinuous. The purpose of this section is to analyze in more detail the distribution of the discontinuity points and the amplitudes of discontinuities of $f(x)$.

Since $f(x)$ is monotone increasing, the amplitudes of its discontinuities are strictly positive. Let us consider a value x_0 of x where $f(x)$ is discontinuous. The amplitude of the corresponding discontinuity is $\delta_0 = f^+(x_0) - f^-(x_0)$ (where $f^+(x)$ and $f^-(x)$ denote the right continuous and left continuous determination of $f(x)$ respectively). Since $g(x) = f(x) - x$ is 2π -periodic, for arbitrary integer m , $f(x)$ also has a discontinuity with the same amplitude δ_0 at

$$x_{0,m} = x_0 + 2m\pi. \quad (21a)$$

Thus in order to fix the ideas, we choose $0 \leq x_0 < 2\pi$. For any $n \in \mathbb{Z}^d$, it is proven [1-3] that $f(x)$ also has discontinuities at

$$x = x_{n,m} = x_0 + nl + 2m\pi \quad (21b)$$

with a strictly positive amplitude δ_n . We set

Definition. The set of discontinuity points $\{x_{n,m}\}$ is called a class of discontinuities \mathcal{D} of the corresponding hull function.

Two classes are either identical or disjoint. Since $f(x)$ is monotone increasing, its set of discontinuities is countable so that there is at most a countable set of disjoint classes \mathcal{D}_i . Using the identity $f(x + 2\pi) = f(x) + 2\pi$, the total variation $V(x_0)$ of $f(x)$ over a period $[0, 2\pi[$ is 2π and thus the variation of $f(x)$ due to the class \mathcal{D} is positive and bounded:

$$V(\mathcal{D}) = \sum_{n \in \mathbb{Z}^d} \delta_n \leq 2\pi = \text{Var}(f(x); [0, 2\pi[). \quad (22a)$$

Since $f(x)$ is a discrete function, the sum of the variation over all classes of discontinuities makes the total variation of $f(x)$ and we have

$$\sum_i V(\mathcal{D}_i) = 2\pi. \quad (22b)$$

For each class, we prove the following theorem:

Theorem 3. Let $f(x)$ be the hull function of an incommensurate ground state of model (1a) with non-zero gap parameter, and $\{x_{n,m}\} = \mathcal{D}$ a class of discontinuities of $f(x)$ as defined by (21b) with amplitudes δ_n . Then the amplitudes of the discontinuities decay exponentially at infinity. More precisely, there exist two positive constants K and γ , such that

$$0 < \delta_n < K \exp(-\gamma|n|) \quad (23)$$

(with $|n| = \sqrt{\sum_{\mu=1}^d n_{\mu}^2}$).

Although this result could reasonably be expected, it is not a straightforward consequence of a positive Lyapunov coefficient (it is not a differential property!) and requires some care for a rigorous proof which is given in appendix E. This proof is based on the following proposition, proven in appendix D, which applies to positive self-adjoint operators on lattices.

Proposition 4. Let us consider a self-adjoint operator $\mathbf{M} = \{M_{i,j}\}$ where the indices $i = \{i_{\tau}\} \in \mathbb{Z}^d$ are the sites of a d -dimensional square lattice. We assume that

$$(i) \quad M_{i,j} = 0 \quad \text{for } |i-j| > p, \quad (24a)$$

$$(ii) \quad M_{i,j} \leq 0 \quad \text{for } i \neq j. \quad (24b)$$

(iii) \mathbf{M} is strictly positive (that is $\langle X|\mathbf{M}|X \rangle > 0$ for any $X \neq 0$).

(iv) Zero does not belong to the spectrum of the operator \mathbf{M} , i.e. the gap parameter of \mathbf{M} is not zero. Let $\mathbf{N} = \{N_{i,j}\} = \mathbf{M}^{-1}$ be the inverse operator, then there exist two positive constants K and γ such that for all $i \in \mathbb{Z}^d$ and $j \in \mathbb{Z}^d$

$$0 < N_{i,j} < K \exp(-\gamma|i-j|). \quad (24c)$$

The same result holds for matrices $\mathbf{M}^{(r)}$, which are defined for $i \in \mathbb{U}$ an arbitrary subset of \mathbb{Z}^d and which fulfill the same conditions.

(Note that if condition (ii) is not fulfilled, $N_{i,j}$ is not necessarily positive but the result (24c) still holds but for $|N_{i,j}|$.) For the FK model (4), numerical calculations have shown that there exists one class of discontinuities. However, we can find an upper bound to the number of classes of discontinuities for a model close to an anti-integrable limit. (See ref. [10], where this concept is described and discussed in detail.) Close to an anti-integrable limit, $L_{\nu}(x, y)$ can be written as

$$L_{\nu}(x, y) = V(x) + C_{\nu} A_{\nu}(x, y), \quad (25)$$

where $V(x)$ is a 2π -periodic twice differentiable function with continuous second-order derivatives and $C_{\nu} A_{\nu}(x, y)$ is the perturbation with amplitude $C_{\nu} \geq 0$. Function $A_{\nu}(x, y)$ has the same properties as those of $L_{\nu}(x, y)$ given in (1). At the anti-integrable limit, obtained for $C_{\nu} \equiv 0$, we have for any stationary configuration $\{u_i\}$, $u_i = a_{\mu_i} + 2m_i\pi$, where m_i is an integer and a_{μ} is one of the solutions of the equation $V'(x) = 0$ with $0 \leq x < 2\pi$. The number of absolute minima of $V(x)$ is generically one.

As suggested by MacKay, we can prove^{#2}.

Theorem 4. When the gap parameter of an incommensurate ground state is not vanishing, the number of discontinuity classes of its hull function is finite.

The proof of this result is based on an idea of MacKay [16]. Assuming that there exists an infinite number of discontinuity classes \mathcal{D}_n , we can find a phase for the incommensurate ground state such that its QEAM exhibits a bounded eigenvector at zero eigenvalue. This fact would imply that the gap parameter of the incommensurate ground state is zero, which contradicts the initial hypothesis and thus proves the theorem.

Thus let us assume that there exists an infinite number of discontinuity classes. Because of inequality (22a) we can choose in each class, a discontinuity point $x_0^{(n)} \in \mathcal{D}_n \cap [0, 2\pi[$ corresponding to the largest amplitude of discontinuity of the hull function $f(x)$: $f^+(x_0^{(n)}) - f^-(x_0^{(n)}) = \sup_{x \in \mathcal{D}_n} [f^+(x) - f^-(x)]$. Considering the set of amplitudes of discontinuity $\{\delta_i^{(n)} = f^+(x_0^{(n)} + i\mathbf{l}) - f^-(x_0^{(n)} + i\mathbf{l})\}$ for $i \in \mathbb{Z}^d$, we define the vector $\{\varepsilon_i^{(n)} = \delta_i^{(n)} / \delta_0^{(n)}\}$ which fulfills for all n and all $i \in \mathbb{Z}^d$: $0 < \varepsilon_i^{(n)} \leq 1$ and $\varepsilon_0^{(n)} = 1$. We now consider an accumulation point $\{x_0, \{\varepsilon_n\}\}$ of the bounded sequence of vectors $\{x_0^{(n)}, \{\varepsilon_i^{(n)}\}\}$ which is limit of the subsequence n_ν . Since the incommensurate ground states $u_i^{(n)+} = f^+(x_0^{(n)} + i\mathbf{l})$ and $u_i^{(n)-} = f^-(x_0^{(n)} + i\mathbf{l})$ both fulfill eq. (2a) and since $\lim_{n \rightarrow \infty} \delta_i^{(n)} = \lim_{n \rightarrow \infty} (u_i^{(n)+} - u_i^{(n)-}) = 0$ and $\lim_{\nu \rightarrow \infty} u_i^{(n_\nu)+} = u_i = f(x_0 + i\mathbf{l})$, where $\{u_i\}$ is an incommensurate ground state, it readily follows that $\{\varepsilon_i\} = \boldsymbol{\varepsilon}$, which fulfills for all i : $0 \leq \varepsilon_i \leq 1$ with $\varepsilon_0 = 1$, is a non-vanishing bounded solution of the eigen-equation $\mathbf{M}(\{u_i\})\boldsymbol{\varepsilon} = 0$. Zero thus should belong to the spectrum of the QEAM of the incommensurate ground state $\{u_i\}$, which contradicts the initial assumption and proves theorem 4.

Close enough to the anti-integrable limit, we also have the more precise theorem:

Theorem 4'. Let us assume that the periodic potential $V(x)$ of the functional (1) at the anti-integrable limit (25) has a single absolute minimum per period, then for any given incommensurate ground state, there exists $C_2 > 0$ such that for $\sup_{\nu \in \mathbb{B}} C_\nu < C_2$ (that is close enough to the anti-integrable limit), there is only one class of discontinuities \mathcal{D} for the hull function of this incommensurate ground state.

Proof. Let us assume first that $V(x)$ has a *single* absolute minimum per period at $x = a \bmod 2\pi$ ($0 \leq a < 2\pi$) and that $V''(a) > 0$. Since $V''(x)$ is continuous, there are two positive constants c and δ such that $V''(x) > c > 0$ for $x \in [a - \delta, a + \delta]$. Then, it can be easily proven that for any ground state configuration $\{u_i\}$, there exists a non-zero constant C_1 such that

$$\sup_{\nu \in \mathbb{B}} C_\nu < C_1 \tag{26a}$$

implies that for all i , there exist m_i such that

$$u_i \in]a - \delta + 2m_i\pi, a + \delta + 2m_i\pi[. \tag{26b}$$

To be more precise, since $\{u_i\}$ is a ground state, the minimum of energy of the potential $V_i(x) = W_i(x) +$

^{#2}This theorem was suggested from R. MacKay's comments.

$V(x)$ where $W_i(x)$ is the potential created by the neighbors of an atom i ,

$$W_i(x) = \sum_{\nu \in \mathbb{B}} C_\nu L_\nu(u_{i+\nu}, x) + \sum_{\nu \in \mathbb{B}} C_\nu L_\nu(x, u_{i-\nu}), \tag{27a}$$

is necessarily obtained for $x = u_i$. A trivial consequence of the existence of the monotone increasing hull function $f(x)$ with $f(x) - x$ 2π -periodic is that $|u_{i+\nu} - u_i - \nu l| < 2\pi$. Function $|L_\nu(x, y)|$, which is “diagonally 2π -periodic” (property (1c)), is bounded by B_ν in the domain mod 2π defined by $|x - y - \nu l|$ (which is compact mod 2π). Thus, in a domain which contains the absolute minimum of $V_i(x)$, we have

$$|W_i(x)| < 2 \sup_{\nu \in \mathbb{B}} |C_\nu| \times \sum_{\nu \in \mathbb{B}} B_\nu = w. \tag{27b}$$

We set

$$v = \inf_{x \in]a+\delta, a-\delta+2\pi[} V(x),$$

which is the minimum of $V(x)$ in the union I of intervals mod 2π , which does not contain the values $a + 2m\pi$, where the absolute minima $V(a)$ is reached; we have $v > V(a)$. Thus by choosing $w < [v - V(a)]/2$ or

$$C_1 = \frac{v - V(a)}{4 \sum_{\nu \in \mathbb{B}} B_\nu} \tag{27c}$$

when (26a) is fulfilled, for $x \in I$, we have $V_i(x) > v - w > V(a) + w$. This result proves that the absolute minimum of $V_i(x)$ is reached for $x = u_i$, which fulfills condition (26b). Then, the “coding sequence” of integers $\{m_i\}$ is determined by the condition that $\{u_i\}$ belongs to the domain $\mathcal{E}(\{m_i\}; \delta)$ of configurations $\{v_i\}$, defined by

$$a - \delta < v_i - 2m_i\pi < a + \delta. \tag{28a}$$

This sequence of integers $\{m_i\}$ is necessarily given by

$$m_i = \text{Int}\left(\frac{u_i - \alpha'}{2\pi}\right) = \text{Int}\left(\frac{f(il + \alpha) - \alpha'}{2\pi}\right), \tag{28b}$$

where α' is an arbitrary number in the interval $[a + \delta - 2\pi, a - \delta]$. Because $f(x)$ is monotonous strictly increasing and because $f(x + 2\pi)/2\pi = f(x)/2\pi + 1$, the integer function $\text{Int}([f(x) - \alpha']/2\pi)$ has a unique discontinuity per period with amplitude 1 for $x = \alpha'' \bmod 1$. Then α'' can be chosen in order that we have

$$\text{Int}\left(\frac{f(x) - \alpha'}{2\pi}\right) = \text{Int}\left(\frac{x - \alpha''}{2\pi}\right). \tag{28c}$$

Thus, we have

$$m_i = \text{Int}\left(\frac{i\ell + \alpha - \alpha''}{2\pi}\right). \tag{28d}$$

Since $V''(x) > c > 0$ for $x \in [a - \delta, a + \delta]$, the Banach fixed point theorem used as explained in ref. [10] allows one to prove that there exists a constant $C_2 \leq C_1$ such that for

$$\sup_{\nu \in \mathbb{B}} |C_\nu| < C_2 \tag{29}$$

the stationary equation (2a) has a unique solution in the domain $\mathcal{E}(\{m_i\}; \delta)$ which has to be the considered ground state $\{u_i\}$.

When condition (29) is fulfilled, suppose that $f(x)$ exhibits a discontinuity for $x = x_0$, then the ground state configurations $\{u_i^+\} = f^+(i\ell - x_0)$ and $\{u_i^-\} = f^-(i\ell - x_0)$ have to be different and thus the corresponding coding sequence of integers $\{m_i\}$

$$m_i^+ = \lim_{x \rightarrow x_0, x > x_0} \text{Int}\left(\frac{i\ell - x - \alpha''}{2\pi}\right), \tag{30a}$$

$$m_i^- = \lim_{x \rightarrow x_0, x < x_0} \text{Int}\left(\frac{i\ell - x - \alpha''}{2\pi}\right) \tag{30b}$$

must be also different. This condition requires that there exists $n \in \mathbb{Z}^d$ such that

$$x_0 = n\ell + \alpha'' \pmod{2\pi}, \tag{30c}$$

which proves that x_0 belongs to the unique class of discontinuities for $f(x)$ generated by α'' . In some cases, $V(x)$ may have several absolute minima per period. Then we only find an upper bound to the number of classes:

When $V(x)$ has r absolute minima per period and close enough to the anti-integrable limit, the hull function has at most r classes of discontinuities.

Let us assume that at the anti-integrable limit $V(x)$ has r absolute minima $V(a_1) = V(a_2) = \dots = V(a_r)$, where $V''(x) > 0$ (we assume $0 \leq a_1 < a_2 < \dots < a_r < 2\pi$). It can be proven on the same footing that close to the anti-integrable limit, the hull functions of the incommensurate ground state have at most r classes of discontinuities. First, we determine $r + 1$ positive constants c and $\{\delta_j\}$ with $j = 1, 2, \dots, r$, such that $V''(x) > c > 0$ for $x \in [a_j - \delta_j, a_j + \delta_j]$. Then, for a given ground state configuration $\{u_i\}$, we prove the existence of a constant C_1 such that for $\sup_{\nu \in \mathbb{B}} C_\nu < C_1$, and for all i , u_i belongs to some interval $[a_j - \delta_j + 2m_i\pi, a_j + \delta_j + 2m_i\pi]$ with m_i an integer. Next, we determine a set of r integers

$$m_i^{(j)} = \text{Int}\left(\frac{u_i - \alpha'_j}{2\pi}\right) = \text{Int}\left(\frac{f(i\ell + \alpha) - \alpha'_j}{2\pi}\right),$$

where α'_j belongs to the interval $]a_j + \delta_j, a_{j+1} + \delta_{j+1}[$ for $j < r$ and to $]a_r + \delta_r, a_1 - \delta_1 + 2\pi[$ for $j = r$. We have for all i , $m_i^{(j)} \leq m_i^{(j+1)}$ for $j < r$ and $m_i^{(r)} \leq m_i^{(1)} + 1$ for $j = r$. With the same argument as for

(28d), there exist r phases α_j'' , with $\alpha_j'' < \alpha_{j+1}''$ and $\alpha_r'' < \alpha_1'' + 2\pi$ such that

$$m_i^{(j)} = \text{Int}\left(\frac{il + \alpha - \alpha_j''}{2\pi}\right).$$

The knowledge of the r sequences $\{m_i^{(j)}\}$ determines unambiguously the location of all the atoms in the intervals $[a_j - \delta_j + 2m_i\pi, a_j + \delta_j + 2m_i\pi]$. For $\sup_{\nu \in \mathbb{B}} C_\nu < C_2 \leq C_1$, the Banach fixed point theorem applied as in ref. [10] proves that the ground state for which the atoms are located in these intervals is unique. The same argument as above allows one to prove that the hull function of this incommensurate ground state has discontinuities only for $x = nl - \alpha_j'' \pmod{2\pi}$. However, the discontinuity classes generated by two different α_j'' may be identical. Thus, this result proves only that there are at most r discontinuity classes.

Although the case where the hull function has a unique discontinuity class seems to occur the most frequently, the hull function may have two and perhaps more discontinuity classes. Particular FK models with the form

$$\Phi(\{u_i\}) = \sum_{\langle i,j \rangle} \frac{1}{2}(u_i - u_j)^2 + \sum_i V(u_i), \tag{31a}$$

where $V(x)$ is a piecewise parabolic 2π -periodic potential with p minima per period with the general form

$$V(x) = \frac{1}{2}k \min_{n=1,2,\dots,p, m \in \mathbb{Z}} [x^2 - 2(a_n + 2m\pi)x + b_n], \tag{31b}$$

where $0 \leq a_n < 2\pi$ are p arbitrary numbers which determine the location of the p minima of $V(x)$ in the first period and b_n are numbers which determine their depth, should provide instructive exactly soluble models where the number of discontinuity classes can be studied easily. (This work has not been done.)

For models which evolve on manifolds in the parameter space such that there are several discontinuity classes for the hull function, the critical behavior at the “breaking of the KAM tori” (for the usual quadratic rotation number) should be changed. This result has to be expected because in a renormalization picture, the fixed point of the renormalization operator corresponding to the large coupling limit (“anti-integrable fixed point”) now depends on the number of discontinuity classes and on their relative weight! Non-universal critical behaviors were indeed observed numerically in models which correspond to this situation [22]. In the next section, we prove that indeed this situation does occur in the examples studied in this reference.

Thus, for a given discontinuity class \mathcal{D} denoted by (21b), we can define the function

$$f_{\mathcal{D}}(x) = \sum_{n \in \mathbb{Z}^d} \delta_n \text{Int}\left(\frac{x - x_0 - nl}{2\pi}\right), \tag{32a}$$

where $\text{Int}(x)$ denotes the largest integer smaller than or equal to x . This series is absolutely convergent since δ_n decays exponentially at infinity (theorem 3). If there is one or a finite number of discontinuity classes, the sum over all discontinuity classes fulfills

$$\sum_{\mathcal{D}} f_{\mathcal{D}}(x) = f(x) + \text{constant}, \tag{32b}$$

since it is a function which has the same amplitude of discontinuity at the same points $x_{n,m}$ as $f(x)$ and since $f(x)$ is a discrete function. The derivative of function $f_{\mathcal{G}}(x)$ considered as a generalized function is

$$\frac{df_{\mathcal{G}}(x)}{dx} = \frac{1}{2\pi} \sum_{n \in \mathbb{Z}^d, m \in \mathbb{Z}} \delta_n \delta(x - x_0 - nl - 2m\pi), \quad (33)$$

where $\delta(x)$ is the Dirac generalized function. Using the identity

$$\frac{1}{2\pi} \sum_{n \in \mathbb{Z}} \delta(x - 2n\pi) = \sum_{m \in \mathbb{Z}} \exp(imx), \quad (34a)$$

we have

$$\frac{df_{\mathcal{G}}(x)}{dx} = \sum_{m \in \mathbb{Z}} h_m \exp[im(x - x_0)] \quad (34b)$$

with

$$h_m = \sum_{n \in \mathbb{Z}^d} \delta_n \exp(-imnl). \quad (34c)$$

Surprisingly, the harmonics of this Fourier series can be described as

$$h_m = h(m), \quad (35a)$$

where $h(x)$ is an 2π -periodic analytic function with Fourier series

$$h(x) = \sum_n \delta_n \exp(-inx). \quad (35b)$$

The analyticity which has been lost for the hull function $f(x)$ at the TBA is restored for the Fourier coefficient of its generalized derivative!

5. Decomposition of an incommensurate ground state into effective discommensurations

Let us assume that an incommensurate ground state of model (1) is described by a discontinuous hull function with a unique class of discontinuities. Since the series $\{\delta_n\}$ is positive and convergent, it is convenient to choose the discontinuity point x_0 (the “origin”) in this class in order that

$$\delta_0 = \sup_{n \in \mathbb{Z}^d} \delta_n. \quad (36a)$$

Using (32a), $\{u_i\}$ is described by

$$u_i = f(il + \alpha) = \sum_n \delta_n \text{Int} \left(\frac{(i-n)l + \alpha - x_0}{2\pi} \right) + \text{const.} \quad (36b)$$

To drop the unknown constant in (36b), it is more convenient to consider the bond lengths

$$x_{i,\mu} = u_i - u_{i-|\mu|} \quad (37a)$$

in the direction μ ($\mu = 1, 2, \dots, d$). In order to fix ideas and without any loss of generality, we assume that for all components μ of $l = \{l_\mu\}$, we have

$$0 \leq l_\mu < 2\pi \quad (l = \{l_\mu\}). \quad (37b)$$

It follows that

$$x_{i,\mu} = f(il + \alpha) - f(il - l_\mu + \alpha) = \sum_m \delta_{i-m} \sigma_{m,\mu} \quad (38a)$$

where the configuration

$$\sigma_{m,\mu} = \chi_\mu(ml + \alpha - x_0) \quad (38b)$$

has the 2π -periodic hull function

$$\chi_\mu(x) = \text{Int}\left(\frac{x}{2\pi}\right) - \text{Int}\left(\frac{x - l_\mu}{2\pi}\right), \quad (38c)$$

which can be chosen to be either left or right continuous. We have for its left continuous determination

$$\chi_\mu(x) = 1 \quad \text{for } 0 \leq x < l_\mu \quad (39a)$$

and

$$\chi_\mu(x) = 0 \quad \text{for } l_\mu \leq x < 2\pi. \quad (39b)$$

Thus when (34b) is fulfilled, $\{\sigma_{m,\mu}\}$ can take only two values, which are 0 or 1, and can be considered as a pseudo-spin configuration.

The bond modulation of the incommensurate ground state, can be described as *the linear superposition* (38a) of localized *effective bond modulations* $\{\delta_n\}$. These local modulations are called “effective discommensurations”. Their distribution is described by d pseudo-spin configuration $\{\sigma_{i,\mu}\}$.

In this case, we assumed (37b) and thus these effective discommensurations refer to the commensurate ground state obtained for $l = 0$. It is essential to note that the shape of a single effective discommensuration depends on the incommensurate ground state (that is on ζ) and thus that *it takes into account the presence of other discommensurations*. According to theorem 3, these effective discommensurations $\{\delta_n\}$ are exponentially localized. For the corresponding ground state, they are located at the bonds where

$$\sigma_{i,\mu} = \chi_\mu(il + \alpha - x_0) = 1. \quad (40a)$$

The size of a discommensuration is defined as the characteristic length ξ associated with the exponential behavior $\exp(-|n|/\xi)$ of δ_n at infinity.

Up to now, the concept of discommensuration was clearly defined [9] only for a single discommensuration and approximately, when these discommensurations are far apart. A single discommensuration is the boundary which separates two regions of a commensurate structure with different phase, for example 0 and 2π for the simplest commensurability $l=0$. It is usually described within the continuous approximation leading to a sine-Gordon model. Within our approach, we obtain a precise definition which applies for many discommensuration structures (many-body problem).

Of course, we also recover the well-known single discommensuration of the ground state obtained for $l=0$, but in addition we take into account the discrete character of the system. The bond modulation associated with a single discommensuration $\{\delta_n\}$ is obtained by taking the limit $l \rightarrow 0$ (and choosing the phase in an appropriate manner [1–3]). At this limit, $\sigma_{i,\mu}$ is zero except on a line of bonds where $\sigma_{i,\mu}$ is only equal to one. These bonds connect two infinite connected regions such that in the first one, the atoms i lie in the interval $[0, 2\pi[$ and in the second one, the atoms lie in $[2\pi, 4\pi[$. The direction of l when it goes to zero determines the direction of the normal vector to the discommensuration. $\{\delta_n\}$ is the bond modulation which allows to know the exact configuration $\{u_i\}$ up to a constant using (36) and the corresponding pseudo-spin configuration.

However, note that in the extended FK models considered in this paper, the pseudo-spin configurations necessarily fulfill the condition

$$\sum_{(i,\lambda) \in \mathcal{C}} s_\lambda \sigma_{i,\lambda} = 0. \quad (40b)$$

The sum of the pseudo-spins is done on any oriented closed loop \mathcal{C} in \mathbb{Z}^d formed by oriented bonds $(i, \lambda = \pm\mu)$ with a weight denoted $s_\lambda = \pm 1$. We have $s_\lambda = 1$, for bonds (i, λ) oriented in the positive direction μ , and $s_\lambda = -1$ for bonds (i, λ) oriented in the negative direction μ . This condition is a severe constraint and implies that the extended FK models in more than one dimension cannot be described by “free” pseudo-spin models. For example, a configuration with a single pseudo-spin equal to one is impossible except for one-dimensional models. This condition originates from the fact that we consider models where atomic vacancies cannot exist. But, let us note that this condition will disappear in coupled electron–phonon models, which otherwise are strongly similar models. They will be studied in ref. [7].

We show in figs. 1 and 2 examples of effective discommensurations which were numerically calculated. For fig. 1, which deals with the standard FK model, there is only one class of discontinuity. It clearly shows that the size of the effective discommensurations diverges when approaching the TBA from above. The example of fig. 2 has been chosen in order that there are two classes of discontinuities. The functional energy (1) of this one-dimensional model is

$$\Phi(\{u_i\}) = \sum_i \left[\frac{1}{2}(u_i - u_{i-1})^2 + V(u_i) \right] \quad (41a)$$

with

$$V(x) = k_1 \cos x + k_2 \cos 2x. \quad (41b)$$

Close to the anti-integrable limit of this model (obtained for large k_1 and k_2 with k_1/k_2 fixed) and when $V(x)$ has two minima per period, according to the result of the previous section, the hull function

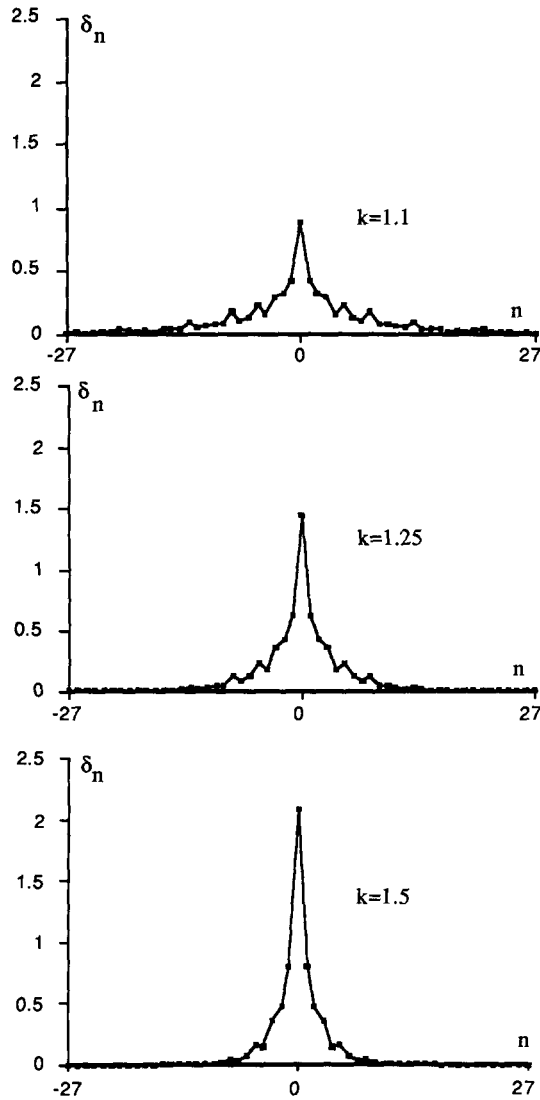


Fig. 1. Three effective discommensurations $\{\delta_n\}$ in the standard FK model (4) (with a unique class of discontinuity) for $\zeta = l/2\pi = \frac{1}{2}(\sqrt{5} - 1)$ and $k = 1.1, 1.25, 1.5$. The size of this discommensuration diverges critically at $k = k_c(\zeta) \cong 0.96$.

of the incommensurate ground state exhibits (at most) two classes of discontinuities. Since we have the symmetry $V(x) = V(-x)$, we can choose the hull function $f(x)$ odd (i.e. fulfilling $f(x) = -f(-x)$). In that case, using theorem 2 in ref. [1], we have $\text{Int}(u_n/\pi) = \text{Int}((nl + \alpha)/\pi)$, which proves that close enough to the anti-integrable limit, $f(x)$ has necessarily a discontinuity at $x = x_0 = 0$ and another one at $x = x_0 = \pi$. These two discontinuities must generate two distinct discontinuity classes.

We calculated the incommensurate ground state for $l/2\pi = \zeta = \frac{1}{2}(\sqrt{5} - 1)$ (the inverse golden mean) and $k_1 = 0.12$ and $k_2 = 0.6$. Then, potential $V(x)$ has two minima per period obtained for $x \cong 1.671$ and $x \cong 4.612$. We observe that $f(x)$ is indeed discontinuous for $x = 0$ and for $x = \pi$. The two sequences δ_n which describe the bond modulation associated with each discommensuration are shown in fig. 1. Note

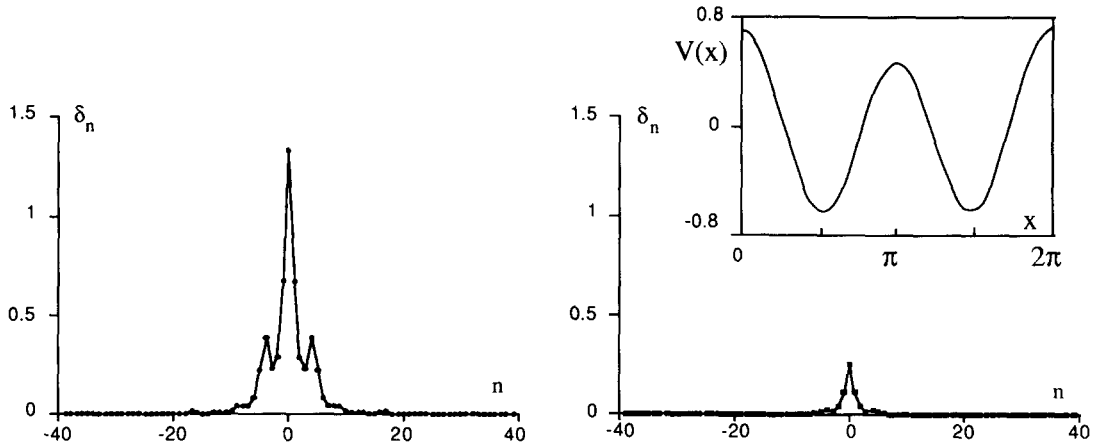


Fig. 2. Example of model (41) with two classes of discontinuity. The two effective discommensurations are shown for $\zeta = l/2\pi = \frac{1}{2}(\sqrt{5} - 1)$, $k_1 = 0.12$ and $k_2 = 0.6$. The graph over a period of potential $V(x)$ is shown in the insert.

that we found for the total amplitude of the first discommensuration $\Delta_1 = \sum_n \delta_n \cong 5.498$, and for those of the second one $\Delta_2 = \sum_n \delta_n \cong 0.785$ (with $\Delta_1 + \Delta_2 \cong 2\pi$). These amplitudes are not apparently related to the distances between the minima of $V(x)$. This very short numerical calculation is just a test for illustrating the present theory. It should be very interesting to explore numerically and to understand better the detailed properties of these effective discommensurations and their possible relation with the critical anomalies at the breaking of the KAM tori observed in ref. [22].

When leaving the anti-integrable limit and approaching the integrable limit at fixed incommensurability ratio ζ , for example by just varying the amplitude of the periodic potential $V(x)$, the incommensurate ground state undergoes a TBA. At this TBA, early studies have shown that the gap parameter Δ and the so-called coherence length ξ are critical [23]. According to theorem 3, the size of the effective discommensuration is identical to the coherence length ξ and thus *diverges* at the TBA. Below the TBA, in the analytic regime (the incommensurate ground state is represented by a KAM torus in the case of the standard FK model), *no effective discommensuration can be defined*. More precisely, since the hull function of the ground state is now analytic, it is impossible to describe the incommensurate ground state as linear superposition of localized lattice distortions since form (38a) would imply a discrete hull function.

We expect that the effective discommensuration of an incommensurate ground state is generally unique unless some specific conditions are required for the model. This effective discommensuration $\{\delta_n\}$ should depend continuously on the incommensurability ratio $\zeta = l/2\pi$ (except when the components of ζ are rationally related!). We expect this result on the basis of results for the 1D nearest-neighbor case [1–3] where the hull function $f(x; \zeta)$ is uniquely defined for ζ irrational (apart from an arbitrary phase shift). Then, we can choose a determination of the phase such that (for most x) we have

$$\lim_{\zeta \rightarrow \zeta_0} f(x; \zeta) = f(x; \zeta_0). \tag{42a}$$

This property implies that for any n , we have

$$\lim_{\zeta \rightarrow \zeta_0} \delta_n(\zeta) = \delta_n(\zeta_0). \tag{42b}$$

When the components of ζ are rational numbers, the hull function $f(x)$ becomes a staircase with a finite number of discontinuities per period. In that case, the effective discommensuration is not uniquely defined by the definition (38). Then, the effective discommensuration $\{\delta_n(\zeta)\}$ might be discontinuous at the points ζ_0 with rational components. We expect that the limit of $\{\delta_n(\zeta)\}$ for $\zeta \rightarrow \zeta_0$ depends on the direction of $(\zeta - \zeta_0)$. However, when the order of commensurability of the rational components of ζ becomes large, these discontinuities become small and negligible. By contrast, we expect that the inverse size $\gamma = 1/\xi$ of these effective discommensurations should vary in rather complex way. It is zero at the values of ζ for which the ground state is analytic but finite non-zero at the rational values. This fact should have potential physical implications for understanding metal–insulator transition in coupled electron–phonon systems as a function of the band filling (or doping).

6. Physical discussion and concluding remarks

This extended definition of a discommensuration is not artificial but should appear to be physically essential for understanding the transport properties and the thermodynamical properties at low temperature of the incommensurate structures with finite gap parameter (which we also called “non-analytic”). Indeed, when the phase $(x_0 - \alpha - n\ell) \bmod 2\pi$ of an incommensurate configuration is changed infinitesimally, this change is associated with the flip of the pseudo-spin n, μ from 0 to 1, and of the pseudo-spin $n - |\mu\rangle, \mu$ from 1 to 0. This phenomenon can be simply viewed as the hopping of an effective discommensuration from the bond $n - |\mu\rangle, \mu$ to the next bond n, μ and only requires a finite displacement of the atoms in a small region of the system. Although this hopping does not cost globally any energy, it requires to overcome the Peierls–Nabarro energy barrier [23]. If the atoms can overcome this energy barrier, the whole system can then be transported.

At 0 K, the “electric field” on the atoms, allowing the global transportation of the system, was calculated in ref. [23] in the standard 1D FK model. With physically reasonable parameter values in the model, the obtained values were found to be physically unrealistic at the macroscopic scale (except very close to the TBA). This result is not very surprising because in real systems, the transport phenomena for a pinned system occur essentially by nucleation and defect transportation (“plastic flow”). At large enough temperature, this motion also becomes possible because it is thermally activated. Then the transport of the whole system under the action of a small electric field is driven by this diffusion process, which occurs at the microscopic scale and is very much temperature dependent. In addition, this diffusive process helps the motions of extra-defects of the structure (e.g. phase domain wall) which should produce non-linear transport phenomena. Such phenomena are indeed commonly observed in CDW systems (e.g. see ref. [8]) which we propose to describe with models with properties similar to those studied here (e.g. see p. 295 in ref. [8]). This problem should also be analyzed in further works with more details on simplified models.

At finite temperature, the thermal fluctuations introduce some disorder in the distribution of the pseudo-spins which describes the location of the effective discommensurations. While the temperature is low enough, the disorder involves defects in the pseudo-spin configuration with a small energy. For example, for the bonds i, μ where the phase $i\ell + \alpha - x_0 \bmod 2\pi$ is slightly larger than zero, the energy cost for flipping an effective discommensuration from bond $i - |\mu\rangle, \mu$ to bond i, μ is not zero but small (e.g. see ref. [24, 25], where this effect is studied on a model in one dimension). The configuration will still be described with a good approximation by a “slightly random” distribution of identical effective discommensurations.

In one-dimensional models, the meaning of “slightly random” can be made more precise by using the concept of word. Indeed, it has been shown in ref. [25] that the pseudo-spin configurations associated with an incommensurate ground state can be constructed following an infinite sequence of two words inflation rules determined explicitly by the continued fraction expansion of the incommensurability ratio $\zeta = l/2\pi$. For example, the special case of the golden mean yields the well-known Fibonacci sequence of words

$$W_n = \{W_{n-1}, W_{n-2}\} \quad (43a)$$

with the initial conditions

$$W_0 = \{0\}, \quad (43b)$$

$$W_1 = \{1\}. \quad (43c)$$

Then, one gets $W_2 = \{10\}$, $W_3 = \{101\}$, $W_4 = \{10110\}$, etc. For n going to infinity, W_n goes to an infinite pseudo-spin sequence which apart from a phase shift is identical to the sequence (40a) with $l = 2\pi\zeta$. An arbitrary configuration of pseudo-spin $\{\sigma_n\}$ referred to the ordered ground state with incommensurability ratio the inverse golden mean $\zeta = \frac{1}{2}(\sqrt{5} - 1)$ is said to be weakly random at order n , when it can be constructed as a random sequence of words W_{n+1} and W_n , the ground state being constructed as an ordered sequences of these two words. This definition can be extended to arbitrary irrational ζ by considering different sequences of words W_n . It has been shown [24, 25] that at low temperature, “non-analytic” 1D incommensurate structures can be well described by weakly random sequences of pseudo-spins at order n . This order n diverges as the temperature goes to zero. Then, the bond modulation of the metastable configurations associated with these weakly random pseudo-spin sequences can be well approximated by (38a) where $\{\delta_i\}$ is the effective discommensuration of the ordered incommensurate ground state. The approximate configuration does not strictly fulfill the stationarity equations (2a). However, in the anti-integrable regime of the Frenkel–Kontorowa model, it can be proven that its uniform distance η_n from the corresponding metastable configuration goes to zero as an exponential of the world length s_n of W_n . (The proof of this result, which is a corollary of the lemma of theorem 8 in ref. [26], should be published later in an extended form.)

Then, pseudo-spin (or integer) models describing weakly random distributions of effective discommensurations naturally appear for modeling the physical behavior of these systems in the “non-analytic incommensurate phases”.

In summary, this paper establishes on a rigorous basis, the existence of effective discommensurations in extended FK models in any dimension at 0 K. It should appear that the existence and the properties of the effective discommensurations are essential features for understanding and predicting the behavior of a “non-analytic” incommensurate structure as a function of temperature and of its transport properties and also for bipolaronic structures as we will see in further works.

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Appendix A. Proof of proposition 1

We prove in fact a more general result valid for any quasi-periodic Hamiltonian and not only for a QEAM.

Let $\mathbf{M}(\alpha)$ be a self-adjoint operator which acts on the vector $X = \{X_i\} \in \mathbb{R}^{\mathbb{Z}^d}$, where the indices $i = \{i_\nu\} \in \mathbb{Z}^d$ are the sites of a d -dimensional square lattice \mathbb{Z}^d . The matrix elements $M_{i,j}(\alpha) = \langle i | \mathbf{M}(\alpha) | j \rangle$ are assumed to be non-zero only for $i = j$ and for close enough sites $\langle i, j \rangle$ on \mathbb{Z}^d with $i - j$ or $j - i \in \mathbb{B}$. They are 2π -periodic functions of a phase α and for any $n \in \mathbb{Z}^d$ for a given vector l in \mathbb{R}^d , we have

$$M_{i,j}(n + \alpha) = M_{i+n,j+n}(\alpha). \quad (\text{A.1a})$$

In addition, these functions of α are left continuous (or right continuous). l is a vector in \mathbb{R}^d with components $\{l_\mu\}$ of this vector which are not rationally related, that is

$$\sum_{\mu=1}^d p_\mu l_\mu \neq 2p\pi \quad (\text{A.1b})$$

for any non-vanishing set of integers $\{p_\mu, p\}$: $\{p_\mu\} \in \mathbb{Z}^d$ and $p \in \mathbb{Z}$. Then, the spectrum of $\mathbf{M}(\alpha)$ does not depend on the phase α

Proof. Since $M_{i,j}(\alpha)$ might be a discontinuous function of the phase α , we cannot even say a priori that the spectrum is a continuous function of α . However, it is obvious that the spectrum of $\mathbf{M}(\alpha)$ is identical to that of $\mathbf{M}(\alpha + nl - 2m\pi)$ for arbitrary $n \in \mathbb{Z}^d$ and $m \in \mathbb{Z}$ because of condition (A.1a) and because $\mathbf{M}(\alpha)$ is 2π -periodic.

By definition, x belongs to the spectrum of $\mathbf{M}(\alpha)$ when $(x\mathbf{I} - \mathbf{M}(\alpha))$ is not invertible in the space of bounded operators (\mathbf{I} is the operator identity). Equivalently, x belongs to the spectrum of $\mathbf{M}(\alpha)$ if and only if there exists a sequence of vectors $X^{(n)}(\alpha)$ such that

$$\lim_{n \rightarrow \infty} \frac{\| [x\mathbf{I} - \mathbf{M}(\alpha)] X^{(n)}(\alpha) \|}{\| X^{(n)}(\alpha) \|} = 0. \quad (\text{A.2a})$$

(Let us recall that the norm used in this definition is the standard Hermitian norm $\|X\| = \sqrt{\sum_i |X_i|^2}$.)

Instead of requiring that vectors $X^{(n)}(\alpha)$ are square summable, it is equivalent to require in (A.2a) that vectors $X^{(n)}(\alpha)$ have a compact support (i.e. the components of $X^{(n)}(\alpha)$ are zero except for the finite set of indices i which belongs to the support).

Let us call \mathbb{S}_N the set of vectors X such that for any i with $|i| = \sup_\nu i_\nu > N$, the vector component X_i is zero. Then, x belongs to the spectrum of $\mathbf{M}(\alpha)$ if and only if there exists a sequence of non-vanishing vectors $X^{(n)}(\alpha)$ which belong to \mathbb{S}_{N_n} for some finite N_n and which fulfill (A.2a). (Note that N_n is not necessarily bounded as a function of n .)

Let us consider a phase α' different from the phase α . We prove that if x belongs to the spectrum of $\mathbf{M}(\alpha)$, it also belongs to the spectrum of $\mathbf{M}(\alpha')$. For that purpose, we construct another sequence of vectors $Y^{(n)}(\alpha')$ such that (A.2a) is also fulfilled for the phase α' .

Let us consider an arbitrary positive number ε . We choose a vector $X^{(n)}(\alpha)$ in the sequence (A.2a) such that

$$\frac{\| [x\mathbf{I} - \mathbf{M}(\alpha)] X^{(n)}(\alpha) \|}{\| X^{(n)}(\alpha) \|} < \frac{1}{2}\varepsilon. \tag{A.2b}$$

Because of (A.1b), there exist sequences $n_p \in \mathbb{Z}^d$ and $m_p \in \mathbb{Z}$ such that

$$\alpha_p = \alpha' + n_p \mathbf{l} - 2m_p \pi \geq \alpha \tag{A.3a}$$

and

$$\lim_{p \rightarrow \infty} \alpha_p = \alpha'. \tag{A.3b}$$

Since $f(x)$ is left continuous, $\lim_{p \rightarrow \infty} M_{i,j}(\alpha_p) = M_{i,j}(\alpha)$ for any i and j . We cannot conclude directly that $\lim_{p \rightarrow \infty} \|\mathbf{M}(\alpha_p) - \mathbf{M}(\alpha)\| = 0$ since the convergence to zero of $|M_{i,j}(\alpha_p) - M_{i,j}(\alpha)|$ for each matrix element does not imply the uniform convergence of the whole operator. However, considering the semi-norm defined as

$$\|M\|_N = \sup_{X \in \mathbb{S}_N} \frac{\|\mathbf{M}X\|}{\|X\|}, \tag{A.4a}$$

where N is such that the chosen vector $X^{(n)}(\alpha)$ in (A.2b) belongs to \mathbb{S}_N . Since this definition only involves finite submatrices of \mathbf{M} , we have

$$\lim_{p \rightarrow \infty} \|\mathbf{M}(\alpha_p) - \mathbf{M}(\alpha)\|_N = 0. \tag{A.4b}$$

Now, we can choose p such that

$$\|\mathbf{M}(\alpha_p) - \mathbf{M}(\alpha)\|_N < \frac{1}{2}\varepsilon. \tag{A.5a}$$

Combining, (A.5a) and (A.2b) yields

$$\begin{aligned} & \frac{\| [x\mathbf{I} - \mathbf{M}(\alpha_p)] X^{(n)}(\alpha) \|}{\| X^{(n)}(\alpha) \|} \\ & \leq \frac{\| [x\mathbf{I} - \mathbf{M}(\alpha)] X^{(n)}(\alpha) \|}{\| X^{(n)}(\alpha) \|} + \frac{\| [\mathbf{M}(\alpha) - \mathbf{M}(\alpha_p)] X^{(n)}(\alpha) \|}{\| X^{(n)}(\alpha) \|} \\ & < \frac{1}{2}\varepsilon + \frac{1}{2}\varepsilon = \varepsilon. \end{aligned} \tag{A.5b}$$

Using (A.1a), we have $M_{i,j}(\alpha_p) = M_{i,j}(\alpha' + n_p \mathbf{l}) = M_{i+n_p, j+n_p}(\alpha')$. Then, considering the vector $Y(\alpha') = \{Y_i\}$ defined as $Y_i = X_{i-n_p}^{(n)}$, (A.5b) becomes

$$\frac{\| [x\mathbf{I} - \mathbf{M}(\alpha')] Y(\alpha') \|}{\| Y(\alpha') \|} < \varepsilon. \tag{A.6}$$

Since for any positive ε , there exists a vector $Y(\alpha')$ which fulfills (A.6), it is clear that a sequence of vectors $Y_n(\alpha')$ can be constructed for a given sequence ε_n converging to zero. Thus, x also belongs to the spectrum of $\mathbf{M}(\alpha')$. Conversely, for any y in the spectrum of $\mathbf{M}(\alpha')$, it can be proven identically that y also belongs to the spectrum of $\mathbf{M}(\alpha)$. The spectrum of $\mathbf{M}(\alpha)$ and $\mathbf{M}(\alpha')$ are thus identical and independent of the phase α , which proves this proposition.

Let us note here that this proof can be extended identically for weakly periodic structures [21]. The important fact in this proof is that any local structure of a configuration for a given “phase” is found again within any arbitrary accuracy in the translated configurations obtained for any other “phase”. For example, the ground state of a model on a square lattice with energy $\sum_{\langle i,j \rangle} L(u_i, u_j)$, where $\langle i, j \rangle$ are nearest-neighbor sites and $L(x, y)$ is only continuous with respect to (x, y) , may be neither periodic (commensurate) nor quasi-periodic (incommensurate). When $L(x, y)$ has neither the property of diagonal periodicity nor the “convexity” property required for the extended FK model, the theories developed in ref. [21] predict that the ground state is necessarily a “weakly periodic” structure. The set $\hat{\mathcal{C}}$ of weakly periodic ground states is then generated from any single ground state $\mathcal{C} = \{u_i\}$ as the closed set of all translated configurations $\{u_{i+p}\}$ for all p and all their limits considered with the weak topology. This set $\hat{\mathcal{C}}$ thus generalizes the concept of phase for an incommensurate structure. Choosing \mathcal{C} in $\hat{\mathcal{C}}$ is analogous to choosing the phase of an incommensurate structure. Then the same proof as above readily extends and allows one to prove that the spectrum of the QEAM of a ground state \mathcal{C} in $\hat{\mathcal{C}}$ is independent of the choice of this ground state \mathcal{C} or in other words of its “phase”.

Appendix B. Proof of proposition 2

We assume that the hull function $f(x)$ of the incommensurate ground state $\{u_i\}$ has a non-constant continuous part $f_c(x) = f_{ac}(x) + f_{sc}(x)$. Since $f(x)$ fulfills the functional equation (10), it comes out that measure $df_c(x)$ is 2π -periodic and fulfills the functional equation obtained by differentiation

$$\begin{aligned} & \sum_{\nu \in \mathbb{B}} \partial_{12} L_\nu(f(x+l_\nu), f(x)) df_c(x+l_\nu) \\ & + \sum_{\nu \in \mathbb{B}} [\partial_{22} L_\nu(f(x+l_\nu), f(x)) + \partial_{11} L_\nu(f(x), f(x-l_\nu))] df_c(x) \\ & + \sum_{\nu \in \mathbb{B}} \partial_{12} L_\nu(f(x), f(x-l_\nu)) df_c(x-l_\nu) = 0. \end{aligned} \quad (\text{B.1})$$

It is easy to prove that $f_c(x)$ is strictly increasing. To prove this result, let us assume that $\int_a^b df_c(x) = 0$ for some couple (a, b) . By integration of (B.1) over the interval $[a, b]$, it follows that

$$\begin{aligned} A = & - \sum_{\nu \in \mathbb{B}} \int_a^b \partial_{12} L_\nu(f(x+l_\nu), f(x)) df_c(x+l_\nu) \\ & - \sum_{\nu \in \mathbb{B}} \int_a^b \partial_{12} L_\nu(f(x), f(x-l_\nu)) df_c(x-l_\nu) = 0. \end{aligned} \quad (\text{B.2a})$$

Condition (1d) implies that the integrands $-\partial_{12} L_\nu(f(x+l_\nu), f(x))$ and $-\partial_{12} L_\nu(f(x), f(x-l_\nu))$ are strictly positive and larger than C for all x . Since each term in the sum (B.2a) is positive or zero, the

equality of their sum to zero implies that each term is zero. Since for all $\nu \in \mathbb{B}$, we have

$$0 = - \int_a^b \partial_{12} L_\nu(f(x + l_\nu), f(x)) df_c(x + l_\nu) \geq C \int_a^b df_c(x + l_\nu) \geq 0, \tag{B.2b}$$

it follows that

$$\int_a^b df_c(x + l_\nu) = \int_{a-l_\nu}^{b-l_\nu} df_c(x) = 0 \tag{B.3a}$$

and

$$\int_a^b df_c(x - l_\nu) = \int_{a+l_\nu}^{b+l_\nu} df_c(x) = 0. \tag{B.3b}$$

Thus the variations of $f_c(x)$ on the intervals $[a \pm l_\nu, b \pm l_\nu] \bmod 2\pi$ are also zero. Then, it is easy to show recursively that the variation of $f_c(x)$ on any interval $[a + \mathbf{p}l + 2p\pi, b + \mathbf{p}l + 2p\pi]$ with $\mathbf{p} = \{p_\nu\} \in \mathbb{Z}^d$ and $p \in \mathbb{Z}$ is zero. Because of condition (5b), these intervals cover the whole real axis, which implies that $df_c(x)$ should be identically zero. This condition contradicts the initial assumption, which proves that when $f_c(x)$ is not a constant, it is a strictly increasing function.

Then it is possible to choose $\zeta = f_c(x)$ as a new variable instead of x . The functions $f(x + nl) = \phi_n(\xi)$ considered as functions of ζ are strictly increasing. According to a theorem of Lebesgue [18], they are differentiable with respect to ξ almost everywhere for the measure $d\xi = df_c(x)$, that is for x belonging to a subset \mathcal{A}_n of \mathbb{R} such that

$$\int_{x \in \mathcal{A}_n \cap [0, 2\pi]} df_c(x) = \int_0^{2\pi} df_c(x). \tag{B.4a}$$

For the countable intersection \mathcal{A} of these supports, \mathcal{A}_n , of the measure $df_c(x)$

$$\mathcal{A} = \bigcap_{n \in \mathbb{Z}^d} \mathcal{A}_n \tag{B.4b}$$

we also have

$$\int_{x \in \mathcal{A} \cap [0, 2\pi]} df_c(x) = \int_0^{2\pi} df_c(x). \tag{B.4c}$$

Therefore, eq. (B.1) shows that for $x \in \mathcal{A}$, the derivative

$$h_n(x) = \frac{df_c(x + nl)}{df_c(x)} \tag{B.5a}$$

is a positive solution of the eigen-equation of the QEAM defined by (6) for the incommensurate ground

state (5a) with phase x

$$\sum_j M_{i,j}(x) h_j(x) \doteq 0. \quad (\text{B.5b})$$

We also have

$$\begin{aligned} \int_0^{2\pi} h_n(x) df_c(x) &= \int_0^{2\pi} \frac{df_c(x+nl)}{df_c(x)} df_c(x) = \int_0^{2\pi} df_c(x+nl) \\ &= \int_{-nl}^{2\pi-nl} df_c(x) = \int_0^{2\pi} df_c(x). \end{aligned} \quad (\text{B.6})$$

The assertions of proposition 2 are now proven.

Appendix C. Proof of proposition 3

We prove in fact a more general result:

Let $\mathbf{M} = \{M_{i,j}\}$ be a self-adjoint operator which acts on the vector space $X = \{X_i\} \in \mathbb{R}^{\mathbb{Z}^d}$ where the indices $i = \{i_\tau\} \in \mathbb{Z}^d$ are the sites of a d -dimensional square lattice. $M_{i,j} = \langle i | \mathbf{M} | j \rangle$ is non-zero only for $i = j$ and for the sites i, j which are connected by a bond in the set \mathbb{B} : $j - i = \pm \nu \in \mathbb{B}$. (The number of connective bonds around each site i is finite and we set $p = \sup_{\nu \in \mathbb{B}} \|\nu\|$ the radius of \mathbb{B} .)

Let us assume that zero does not belong to the spectrum of the operator \mathbf{M} and that $\{\Psi_i\}$ is a solution of the eigen-equation at zero eigenvalue.

$$\sum_j M_{i,j} \Psi_j = 0 \quad \text{for all } i. \quad (\text{C.1a})$$

We define for $n \geq 0$

$$A_n = \sum_{i \in \mathbb{D}_n} |\Psi_i|^2 \quad (\text{C.1b})$$

where \mathbb{D}_n are the sites $i = \{i_\tau\}$ fulfilling $\max_\tau |i_\tau| = \|i\| = n$. These sites form the boundary of the cube \mathbb{K}_n defined by $\max_\tau |i_\tau| = \|i\| \leq n$.

Then A_n diverges exponentially for n going to infinity when the gap parameter $\Delta = 1/\|\mathbf{M}\| \|\mathbf{M}^{-1}\|$ of \mathbf{M} is non-vanishing. More precisely, we have the following bound for all $n > 1$:

$$K \exp(\gamma n) < A_n, \quad (\text{C.2a})$$

where the constant γ , which is non-vanishing, only depends on this gap parameter and on the connectivity set \mathbb{B} and the dimensionality of the model while the constant K although non-vanishing, may depend on the solution $\{\Psi_i\}$.

Proof. Since zero does not belong to the spectrum of \mathbf{M} , then \mathbf{M} is invertible and $\|\mathbf{M}^{-1}\|$ is finite. Thus, for any vector $\phi = \{\phi_i\}$, we have with $\phi' = \mathbf{M} \cdot \phi$

$$\frac{\|\mathbf{M} \cdot \phi\|}{\|\phi\|} = \frac{\|\phi'\|}{\|\mathbf{M}^{-1} \cdot \phi'\|} \geq \inf_{\phi'} \frac{\|\phi'\|}{\|\mathbf{M}^{-1} \cdot \phi'\|} = \frac{1}{\|\mathbf{M}^{-1}\|} \quad (\text{C.3a})$$

or

$$\|\mathbf{M} \cdot \phi\| \geq \frac{1}{\|\mathbf{M}^{-1}\|} \|\phi\|. \quad (\text{C.3b})$$

For $n > 0$, let us now choose the particular vector $\{\phi_i\}$ defined as

$$\phi_i = \psi_i \quad \text{for } i \in \mathbb{K}_n \quad (\text{C.4a})$$

and

$$\phi_i = 0 \quad \text{for } i \notin \mathbb{K}_n. \quad (\text{C.4b})$$

Because of (C.3b), we have

$$\|\mathbf{M} \cdot \phi\|^2 \geq \frac{1}{\|\mathbf{M}^{-1}\|^2} \sum_{i \in \mathbb{K}_n} |\psi_i|^2. \quad (\text{C.5})$$

Using (C.1) and (C.4) and the fact that $M_{i,j} = 0$ when i and j are not identical and $\pm(i-j) \in \mathbb{B}$ yields that

(1) for $i \in \mathbb{K}_{n-p}$ and for $i \notin \mathbb{K}_{n+p}$, we have

$$(\mathbf{M} \cdot \phi)_i = 0; \quad (\text{C.6a})$$

(2) for i close enough to the boundary of \mathbb{K}_n , that is for $i \in \mathbb{K}_{n+p} - \mathbb{K}_{n-p}$,

$$(\mathbf{M} \cdot \phi)_i = \sum_{j \in \mathbb{K}_n} M_{i,j} \psi_j \neq 0. \quad (\text{C.6b})$$

Since the maximum number of sites j connected to a site i by a bond in \mathbb{B} is $(2p+1)^d$, we have the inequality

$$|(\mathbf{M} \cdot \phi)_i|^2 = \left| \sum_j M_{i,j} \psi_j \right|^2 \leq (2p+1)^{2d} \sum_j |M_{i,j} \psi_j|^2. \quad (\text{C.7a})$$

Using the trivial property $|M_{i,j}| < \|\mathbf{M}\|$, we obtain for $n > 0$

$$\begin{aligned} \|\mathbf{M} \cdot \phi\|^2 &= \sum_{i \in \mathbb{K}_{n+p} - \mathbb{K}_{n-p}} (\mathbf{M} \cdot \phi)_i^2 < (2p+1)^{2d} \sup |M_{i,j}|^2 \times \sum_{i \in \mathbb{K}_{n+p} - \mathbb{K}_{n-p}} |\psi_i|^2 \\ &< (2p+1)^{2d} \|\mathbf{M}\|^2 \sum_{-p < j \leq p} \sum_{i \in \mathbb{D}_{n+j}} |\psi_i|^2. \end{aligned} \quad (\text{C.7b})$$

(C.5) and (C.7b) yield

$$\sum_{i \in \mathbb{K}_n} |\Psi_i|^2 < (2p + 1)^{2d} \|\mathbf{M}^{-1}\|^2 \|\mathbf{M}\|^2 \sum_{i \in \mathbb{D}_{n+i}} |\Psi_i|^2. \tag{C.8a}$$

Using the definition (C.1b), (C.8a) becomes

$$c \sum_{i=0}^n A_i < \sum_{-p < j \leq p} A_{n+j}, \tag{C.8b}$$

where the constant c is

$$c = \frac{\Delta^2}{(2p + 1)^{2d}}. \tag{C.8c}$$

For $n \geq p$, this positive sequence A_n is necessarily larger than the positive and monotonically increasing sequence a_n generated by

$$c \sum_{i=0}^n a_i = \sum_{-p < j \leq p} a_{n+j} \tag{C.9a}$$

with the initial conditions $a_n = A_n > 0$ for $n \leq p$.

Considering eq. (C.9a) obtained by changing n into $n - 1$

$$c \sum_{i=0}^{n-1} a_i = \sum_{-p < j \leq p} a_{n-1+j}, \tag{C.9b}$$

one obtains by comparing (C.9a) and (C.9b)

$$ca_n = a_{n+p} - a_{n-p}. \tag{C.9c}$$

For a given $n \leq p$, the sequence $b_i = a_{n+ip}$ fulfills the recursive relation $b_{i+1} = cb_i + b_{i-1}$. The characteristic matrix of this recursion relation $\begin{pmatrix} c & 1 \\ 1 & 0 \end{pmatrix}$ with determinant -1 , has two real eigen-values $y > 1$:

$$y = \frac{1}{2}c + \frac{1}{2}\sqrt{c^2 + 4} = \exp(p\gamma) > 1 + \frac{1}{2}c > 1 \tag{C.10a}$$

and $-y^{-1}$. $\gamma > 0$ only depends on c and p but is independent on the solution Ψ_i . Since its initial conditions are always positive, this sequence $b_i = a_{n+ip}$ always diverges exponentially as y^i and since the second eigenvalue of the characteristic matrix has a modulus strictly smaller than 1, there exists a non-vanishing constant K_n such that $b_i > K_n y^i = N_n \exp(-n\gamma) \exp[(ip + n)\gamma]$. Thus, there also exists a *non-vanishing* constant $K = \text{Inf}_{0 < n \leq p} [K_n \exp(-n\gamma)]$ which depends on the initial values of A_n such that for all m we have

$$K \exp(m\gamma) < a_m < A_m, \tag{C.10b}$$

which proves proposition 3.

Appendix D. Proof of proposition 4

The proof of this proposition requires different hypotheses from those of appendix C. We first write the identity

$$\mathbf{M} = \|\mathbf{M}\|(\mathbf{I} - \mathbf{B}) \quad (\text{D.1a})$$

with

$$\mathbf{B} = \mathbf{I} - \frac{\mathbf{M}}{\|\mathbf{M}\|}. \quad (\text{D.1b})$$

Since operator \mathbf{M} is strictly positive, the upper bound of the spectrum of \mathbf{M} is $\|\mathbf{M}\|$ and its lower bound is $1/\|\mathbf{M}^{-1}\|$. Thus, the whole spectrum of \mathbf{B} defined by (D.1b) belongs to the interval $[0, 1 - 1/\|\mathbf{M}\| \|\mathbf{M}^{-1}\|]$ and consequently, we have

$$\|\mathbf{B}\| = 1 - \frac{1}{\|\mathbf{M}\| \|\mathbf{M}^{-1}\|} = 1 - \Delta < 1. \quad (\text{D.2a})$$

As a result, \mathbf{B} is a strictly positive operator with a norm strictly smaller than 1. This condition implies $B_{i,i} \geq 0$ for all i . Since $B_{i,j} = \delta_{i,j} - M_{i,j}/\|\mathbf{M}\|$, we also have for $i \neq j$

$$B_{i,j} \geq 0. \quad (\text{D.2b})$$

In addition, we have

$$B_{i,j} = 0 \quad \text{for all } i, j \in \mathbb{Z}^d \quad \text{such that } |i - j| > p = \sup_{\nu \in \mathbb{B}} \|\nu\| \quad (\text{D.2c})$$

(the bond interaction). Since $\|\mathbf{B}\| < 1$, we can write the inverse \mathbf{M}^{-1} as a convergent series of operators

$$\mathbf{N} = \mathbf{M}^{-1} = \frac{1}{\|\mathbf{M}\|} \sum_{n=0}^{+\infty} \mathbf{B}^n. \quad (\text{D.3a})$$

Since the coefficients $B_{i,j}$ are all positive or zero, the coefficients $(\mathbf{B}^n)_{i,j}$ are also positive or zero. In addition, using the fact that $B_{k,j} = 0$ for $|k - j| > p$ and the recursion relation

$$(\mathbf{B}^n)_{i,j} = \sum_k (\mathbf{B}^{n-1})_{i,k} B_{k,j} \quad (\text{D.3b})$$

we find recursively that

$$(\mathbf{B}^n)_{i,j} = 0 \quad \text{for } |i - j| > np. \quad (\text{D.4a})$$

We have

$$0 \leq (\mathbf{B}^n)_{i,j} \leq \|\mathbf{B}^n\| \leq \|\mathbf{B}\|^n \leq (1 - \Delta)^n \quad \text{for } |i - j| \leq np. \quad (\text{D.4b})$$

Then, it follows that

$$\begin{aligned} 0 < N_{i,j} &= \frac{1}{\|\mathbf{M}\|} \sum_{n \geq |i-j|/p} (\mathbf{B}^n)_{i,j} \leq \frac{1}{\|\mathbf{M}\|} \sum_{n \geq |i-j|/p} (1-\Delta)^n \\ &= \frac{1}{\Delta \|\mathbf{M}\|} (1-\Delta)^{|i-j|/p} = K \exp(-\gamma|i-j|), \end{aligned} \quad (\text{D.5a})$$

which proves proposition 4 for

$$K = (\Delta \|\mathbf{M}\|)^{-1} = \|\mathbf{M}^{-1}\| \quad (\text{D.5b})$$

and

$$\gamma = -p^{-1} \ln(1-\Delta) > 0. \quad (\text{D.5c})$$

Appendix E. Proof of theorem 3

The hull function $f(x)$ being discontinuous for $x = x_0$, we consider the two incommensurate ground state configurations defined as

$$u_i^+ = f^+(il - x_0), \quad (\text{E.1a})$$

$$u_i^- = f^-(il - x_0), \quad (\text{E.1b})$$

where $f^+(x)$ and $f^-(x)$ are the right continuous and the left continuous determinations of the hull function respectively. Then, we have

$$u_i^+ - u_i^- = \delta_{-i}, \quad (\text{E.1c})$$

where δ_{-i} is the amplitude of discontinuity of $f(x)$ at $x_{-i} = -il + x_0$ defined in (21). These two configurations $\{u_i^+\}$ and $\{u_i^-\}$ fulfill eq. (2a)

$$\sum_{\nu \in \mathbb{B}} \partial_2 L_\nu(u_{i+\nu}^+, u_i^+) + \sum_{\nu \in \mathbb{B}} \partial_1 L_\nu(u_i^+, u_{i-\nu}^+) = 0 \quad (\text{E.2a})$$

and

$$\sum_{\nu \in \mathbb{B}} \partial_2 L_\nu(u_{i+\nu}^-, u_i^-) + \sum_{\nu \in \mathbb{B}} \partial_1 L_\nu(u_i^-, u_{i-\nu}^-) = 0. \quad (\text{E.2b})$$

Since functions $L_\nu(x, y)$ have continuous second-order derivatives, for each bond, (i, ν) (or $(i, -\nu)$), there exists a couple of numbers $(\xi_{i,\nu}, \eta_{i,\nu})$ (or $(\xi_{i,-\nu}, \eta_{i,-\nu})$) which fulfill the inequalities

$$u_i^- \leq \xi_{i,\nu} \leq u_i^+ \quad \text{and} \quad u_{i+\nu}^- \leq \eta_{i,\nu} \leq u_{i+\nu}^+, \quad (\text{E.3a})$$

$$u_i^- \leq \xi_{i,-\nu} \leq u_i^+ \quad \text{and} \quad u_{i-\nu}^- \leq \eta_{i,-\nu} \leq u_{i-\nu}^+ \quad (\text{E.3b})$$

and

$$\begin{aligned} & \partial_2 L_\nu(u_{i+\nu}^+, u_i^+) - \partial_2 L_\nu(u_{i+\nu}^-, u_i^-) \\ &= (u_i^+ - u_i^-) \partial_{22} L_\nu(\eta_{i,\nu}, \xi_{i,\nu}) + (u_{i+\nu}^+ - u_{i+\nu}^-) \partial_{21} L_\nu(\eta_{i,\nu}, \xi_{i,\nu}) \\ &= \delta_{-i} \partial_{22} L_\nu(\eta_{i,\nu}, \xi_{i,\nu}) + \delta_{-(i+\nu)} \partial_{21} L_\nu(\eta_{i,\nu}, \xi_{i,\nu}), \end{aligned} \quad (\text{E.4a})$$

$$\begin{aligned} & \partial_1 L_\nu(u_i^+, u_i^{+\nu}) - \partial_1 L_\nu(u_i^-, u_i^{-\nu}) \\ &= (u_i^+ - u_i^-) \partial_{11} L_\nu(\xi_{i,-\nu}, \eta_{i,-\nu}) + (u_{i-\nu}^+ - u_{i-\nu}^-) \partial_{12} L_\nu(\xi_{i,-\nu}, \eta_{i,-\nu}) \\ &= \delta_{-i} \partial_{11} L_\nu(\xi_{i,-\nu}, \eta_{i,-\nu}) + \delta_{-(i-\nu)} \partial_{12} L_\nu(\xi_{i,-\nu}, \eta_{i,-\nu}). \end{aligned} \quad (\text{E.4b})$$

Then by difference of the first members of eqs. (E.2), we obtain

$$\sum_j P_{i,j} \delta_{-j} = 0, \quad (\text{E.5a})$$

where the infinite matrix $\mathbf{P} = \{P_{i,j}\}$ is defined as

$$P_{i,i} = \partial_{11} L_\nu(\xi_{i,-\nu}, \eta_{i,-\nu}) + \partial_{22} L_\nu(\eta_{i,\nu}, \xi_{i,\nu}), \quad (\text{E.5b})$$

$$P_{i,j} = \partial_{12} L_\nu(\xi_{i,-\nu}, \eta_{i,-\nu}) \quad \text{when } \nu = i - j \in \mathbb{B}, \quad (\text{E.5c})$$

$$P_{i,j} = \partial_{21} L_\nu(\eta_{i,\nu}, \xi_{i,\nu}) \quad \text{when } \nu = j - i \in \mathbb{B}, \quad (\text{E.5d})$$

$$P_{i,j} = 0 \quad \text{when } i - j \notin \mathbb{B} \quad \text{and} \quad j - i \notin \mathbb{B}. \quad (\text{E.5e})$$

Since δ_i is positive and the series $\sum_{i \in \mathbb{Z}^d} \delta_i \leq 2\pi$ convergent, we have

$$\lim_{|i| \rightarrow \infty} \delta_i = 0 \quad (\text{E.6a})$$

and consequently

$$\lim_{|i| \rightarrow \infty} (\xi_{i,\nu} - u_i^-) = \lim_{|i| \rightarrow \infty} (\xi_{i,\nu} - u_i^-) = 0, \quad (\text{E.6b})$$

$$\lim_{|i| \rightarrow \infty} (\eta_{i,\nu} - u_{i+\nu}^-) = \lim_{|i| \rightarrow \infty} (\eta_{i,-\nu} - u_{i-\nu}^-) = 0. \quad (\text{E.6c})$$

Since the second-order derivatives of $L_\nu(x; y)$ are supposed to be uniformly continuous functions of (x, y) for $|\nu| \leq p$, we have the *uniform* limit

$$\lim_{\substack{|i| \rightarrow \infty \\ |j| \rightarrow \infty}} |P_{i,j} - M_{i,j}| = 0, \quad (\text{E.6d})$$

where $\mathbf{M} = \{M_{i,j}\}$ is the QEAM of configuration $\{u_i^-\}$.

Let us now define the truncated infinite matrices $\mathbf{M}^{(r)}$ and $\mathbf{P}^{(r)}$ which are self-adjoint operators in the subspace $\mathbb{E}^{(r)}$ of states spanned by the basis of all vectors $|i\rangle$ with $|i| \geq r$. (For $r = 0$, $\mathbb{E}^{(0)}$ is the full space.)

Since operator \mathbf{M} and its submatrices $\mathbf{M}^{(r)}$ are positive, their spectral norms $\|\mathbf{M}\|$ and $1/\|\mathbf{M}^{-1}\|$, which are equivalently defined by (8b) and (8c), fulfill

$$\|\mathbf{M}^{(r)}\| = \sup_{0 \neq X \in \mathbb{E}^{(r)}} \frac{\langle X | \mathbf{M} | X \rangle}{\langle X | X \rangle} \leq \sup_{X \neq 0} \frac{\langle X | \mathbf{M} | X \rangle}{\langle X | X \rangle} = \|\mathbf{M}\|, \quad (\text{E.7a})$$

which is the infimum of the spectrum of \mathbf{M} , as

$$\frac{1}{\|\mathbf{M}^{(r)-1}\|} = \inf_{0 \neq X \in \mathbb{E}^{(r)}} \frac{\langle X | \mathbf{M} | X \rangle}{\langle X | X \rangle} \geq \inf_{X \neq 0} \frac{\langle X | \mathbf{M} | X \rangle}{\langle X | X \rangle} = \frac{1}{\|\mathbf{M}^{-1}\|}. \quad (\text{E.7b})$$

Since each site i is connected at most to $(2p + 1)^d$ sites j , each line or column of $\mathbf{M}^{(r)}$, $\mathbf{P}^{(r)}$ and $\mathbf{M}^{(r)} - \mathbf{P}^{(r)}$ contains at most $(2p + 1)^d$ terms which are non-zero. Consequently, we have the inequality

$$N_r = \|\mathbf{M}^{(r)} - \mathbf{P}^{(r)}\| \leq (2p + 1)^d \sup_{|i| \geq r, |j| \geq r} |P_{i,j} - M_{i,j}| \quad (\text{E.8a})$$

for the spectral norm of operators $\|\cdot\|$. Since the limit (E.6d) is uniform, N_r goes to zero for $r \rightarrow \infty$, and we can choose r large enough, in order that we have the strict inequality

$$\|\mathbf{M}^{(r)} - \mathbf{P}^{(r)}\| = N_r < 1/\|\mathbf{M}^{-1}\|. \quad (\text{E.8b})$$

The lower bound of the spectrum of $\mathbf{M}^{(r)}$ is larger than $1/\|\mathbf{M}^{-1}\|$ so that this condition (E.8b) implies that the spectrum of operator $\mathbf{P}^{(r)}$ is also strictly positive. We also have

$$\begin{aligned} \frac{1}{\|\mathbf{P}^{(r)-1}\|} &= \inf_{X \in \mathbb{E}^{(r)}} \frac{\|\mathbf{P}^{(r)} X\|}{\|X\|} = \inf_{X \in \mathbb{E}^{(r)}} \frac{\|[(\mathbf{P}^{(r)} - \mathbf{M}^{(r)}) + \mathbf{M}^{(r)}] X\|}{\|X\|} \\ &\geq \inf_{X \in \mathbb{E}^{(r)}} \frac{\|\mathbf{M}^{(r)} X\|}{\|X\|} - \sup_{X \in \mathbb{E}^{(r)}} \frac{\|(\mathbf{P}^{(r)} - \mathbf{M}^{(r)}) X\|}{\|X\|} \\ &> \frac{1}{\|\mathbf{M}^{(r)-1}\|} - \|(\mathbf{P}^{(r)} - \mathbf{M}^{(r)})\| > \frac{1}{\|\mathbf{M}^{-1}\|} - N_r > 0, \end{aligned} \quad (\text{E.9a})$$

which implies that the gap parameter of $\mathbf{P}^{(r)}$ fulfills

$$\Delta_r = \frac{1}{\|\mathbf{P}^{(r)}\| \|\mathbf{P}^{(r)-1}\|} > \Delta - \frac{N_r}{\|\mathbf{M}\|} > 0, \quad (\text{E.9b})$$

where Δ is the gap parameter of \mathbf{M} .

We now note that eq. (E.5a) can also be written as

$$\mathbf{P}^{(r)} \cdot \Delta_r = B_r, \quad (\text{E.10a})$$

where Δ_r, B_r are vectors defined for $|i| \geq r$ as

$$(\Delta_r)_i = \{\delta_{-i}\}, \quad (\text{E.10b})$$

$$(B_r)_i = - \sum_{|j| < r} P_{i,j} \delta_{-j} \geq 0. \quad (\text{E.10c})$$

Δ_r is square summable because the positive series $\sum_{i \in \mathbb{Z}^d} \delta_i$ is convergent. We note that only a finite

number of components of \mathbf{B}_r are non-zero since

$$(\mathbf{B}_r)_i = 0 \quad \text{for } |i| \geq r + p. \quad (\text{E.11a})$$

\mathbf{B}_r and Δ_r both belong to the Hilbert space $\mathbb{E}^{(r)}$. Since operator $\mathbf{P}^{(r)}$ is invertible in this space $\mathbb{E}^{(r)}$, we have

$$\Delta_r = \mathbf{P}^{(r)-1} \cdot \mathbf{B}_r. \quad (\text{E.11b})$$

It fulfills the hypothesis of proposition 4, which yields for $|i| \geq r$

$$0 < \delta_{-i} < K_r \sum_{|j| < p+r} \exp(-\gamma_r|i-j|) (\mathbf{B}_r)_j \quad (\text{E.12a})$$

with

$$K_r = \|\mathbf{P}^{(r)-1}\| \quad (\text{E.12b})$$

and

$$\gamma_r = -\frac{1}{p} \ln \Delta_r = -\frac{1}{p} \ln \left(\Delta - \frac{N_r}{\|\mathbf{M}\|} \right). \quad (\text{E.12c})$$

Theorem 3 is proven with constants K and γ in (23) defined as

$$K = \sup \left(\sup_{i < r} \delta_i \exp(\gamma|i|), K_r \sum_{|j| < r+p} \exp(\gamma_r|j|) (\mathbf{B}_r)_j \right) > 0 \quad (\text{E.13})$$

and $\gamma = \gamma_r$.

Let us note that N_r can be small, which shows that this coefficient γ_r can be chosen very close to that of \mathbf{M} . (However, the constant K might become very large.) Thus in the case when a twist map can be associated with the variational form (1), γ can be indeed chosen very close to the Lyapunov coefficient of the trajectory corresponding to the incommensurate ground states.

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