

# Resonance and non-recurrent rotationally ordered configuration in Frenkel-Kontorova models

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**Abstract.** We demonstrate, with a class of exactly solvable Frenkel-Kontorova models, the emergence of the non-recurrent rotationally ordered configurations whenever certain resonance conditions are satisfied among the openings in the hull function in both the commensurate and the incommensurate cases. If one insists on depicting them with hull functions, suitably defined extended numbers must be employed. The defect-mediated transition in the incommensurate case is also discussed.

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## 1 Introduction

Mode locking to commensurate ratios of parameters is a common phenomenon in nonlinear dynamics and condensed matter physics [1]. The Frenkel-Kontorova (FK) model and its accompanying two-dimensional area-preserving twist map is among the simplest examples to reveal such nontrivial phenomenon. This model describes a linear chain of coupled atoms in an external periodic potential. The energy of the system has the form

$$H(\mathbf{u}) = \sum_n \left[ \frac{1}{2} (u_{n+1} - u_n)^2 + \lambda V(u_n) \right], \quad (1)$$

where  $u_n$  is the position of the  $n$ th atom and  $\mathbf{u}$  denotes the bi-infinite sequence  $\{\dots, u_n, \dots\}$ . The periodic potential  $\lambda V(u)$  has amplitude  $\lambda$  and period  $l$ , which can be set to 1 with a suitable choice of the length scale. For a stationary configuration one has  $\partial H / \partial u_n = 0$  and thus

$$u_{n+1} - 2u_n + u_{n-1} = \lambda V'(u_n), \quad (2)$$

which can be formulated as a two-dimensional area-preserving twist map defined on the cylinder  $[0, 1) \times \mathbf{R}$  [2, 3].

In Aubry's terminology [4], a minimum energy configuration  $\mathbf{u}$  is one in which  $H$  cannot be decreased by altering a finite number of  $u_n$ . Alternatively,  $\mathbf{u}$  is said to minimize the energy if, for every bi-infinite sequence  $\mathbf{v} \equiv \{\dots, v_n, \dots\}$  such that  $\sum_{n=-\infty}^{\infty} |u_n - v_n| < \infty$ , one has

$$\sum_{n=-\infty}^{\infty} [h(v_n, v_{n+1}) - h(u_n, u_{n+1})] \geq 0, \quad (3)$$

where  $h(u, v) \equiv [(u - v)^2 + V(u) + V(v)]/2$ , and the sum on the left is absolutely convergent [5]. For the  $h$  function satisfying some conditions (which were generalized by Bangert [5, 6]), the minimum energy configurations must observe the celebrated *Aubry's crossing lemma* (called the fundamental lemma in [4]) [7]. Under this circumstance, there is a well-defined winding number

$$\omega = \lim_{N, N' \rightarrow \infty} \frac{u_N - u_{-N'}}{N + N'}, \quad (4)$$

which is also the mean atomic distance.

In terms of dynamical systems, the minimum energy configurations correspond to the (action) minimizing orbits of the twist map defined on a cylinder [3, 5]. Let  $\Sigma$  denote the set of all the minimizing orbits,  $\Sigma_\omega$  denote the subset of  $\Sigma$  consisting of minimizing orbits of winding number  $\omega$ , and  $\Sigma_\omega^*$  denote the minimizing orbits for the winding number  $\omega$  (which, in fact, correspond to the ground state configurations). For a generic area-preserving twist map,  $\Sigma_\omega = \Sigma_\omega^*$  for irrational  $\omega$  and  $\Sigma_\omega^* \subset \Sigma_\omega$  for rational  $\omega$  [5]. In the latter case,  $\Sigma_\omega^*$  consists of a single periodic orbit, but according to the Aubry-Le Daeron theory [4],  $\Sigma_\omega$  contains other orbits as well, which are *non-recurrent* and are heteroclinic to the orbit in  $\Sigma_\omega^*$ . For an orbit to be *recurrent*, every point of the orbit defined on the cylinder must have points of the orbit, after some forward or backward iterations of mapping, arbitrarily close to it. For rational  $\omega = p/q$  (all fractions are assumed to be irreducible throughout this paper), the orbit in  $\Sigma_\omega^*$  will take the same point after every  $q$  times of mapping, so the orbit is not only recurrent but also *repetitious*.

Recently, Griffiths *et al.* found, in a general class of exactly solvable FK models, that non-recurrent minimizing orbits, which are *homoclinic* to the corresponding

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recurrent orbits in  $\Sigma_\omega^*$ , could exist even in the incommensurate case [8].

A ground state is by definition a recurrent minimum energy configuration, whose atomic positions can be characterized by [4]

$$u_n = f_\omega(n\omega + \alpha). \quad (5)$$

Here the hull function  $f_\omega(x)$  is increasing and satisfies

$$f_\omega(x + 1) = f_\omega(x) + 1, \quad (6)$$

and  $\alpha$  is a phase variable which determines the relative position of the atomic chain with respect to the periodic potential. As  $\lambda$  increases, the plot of the orbit (defined on a cylinder) for an incommensurate ground state undergoes a transition from a KAM invariant curve, corresponding to an unpinned phase, to a Cantor-Aubry-Mather (CAM) set [9] or a cantor, corresponding to a pinned phase. In the latter case  $f_\omega(x)$  fails to be a continuous function, the positions of the atoms can be depicted by choosing the righthand side limit  $f_\omega^r(x)$  or the lefthand side one  $f_\omega^l(x)$ . The transition, featured by the breaking of the KAM invariant curve, is termed “the transition by breaking of analyticity” (TBA) [1,2,4]. We are particularly interested in the structure of the cantor and its relation to the non-recurrent configurations in the present work.

The above mentioned properties of minimum energy configuration stem from the fact that, after TBA, the minimizing orbits still mimic the invariant curves to be *rotationally ordered* (RO) [10–12] (called *special* in [13]). More specifically, let us introduce the shift operation to include the shifts in the  $u$ -axis by integers (periods of potential) or in the numbering of atoms. Aubry’s crossing lemma guarantees the ground state or minimum energy configurations not to *self-intersect*, *i.e.*, not to intersect, unless coincide with, its own shifts (by applying the shift operation to itself). Two configurations  $\mathbf{u}$  and  $\mathbf{v}$  are said to *intersect* if there are  $u_n \geq v_n$  and  $u_m \leq v_m$  for some  $n$  and  $m$ . While, they are said to coincide if  $u_n = v_n$  for every  $n$ .

Without referring to the concept of ground state or minimum energy configurations, which are of central concern in condensed matter physics, the set of all the RO orbits should have its own significance in dynamical systems since they are all remnants of the KAM invariant curves and should all play the role of partial barrier to the transport in phase space [14].

After TBA, the hull function is purely discrete [9]. Thus there must be discontinuities (called *gaps*) in the hull function. The gaps must come in orbits; that is, if there is a gap of  $f_\omega(x)$  at  $x = \beta$ , then there is a class of gaps (called a *hole*) at  $x = \text{Frac}[\beta + n\omega]$  for all integers  $n$  with  $\text{Frac}[x] = x - \text{Int}[x]$  denoting the fractional part of  $x$ . In the anti-integrability limit and in numerical simulation, it was found that there might be more than one hole in the minimizing orbits [9–11]. To be more specific, the right-end (left-end) points of all the gaps belonging to a specific hole would compose one of the minimizing orbits, which can be depicted by the hull function  $f_\omega^r(x)$  ( $f_\omega^l(x)$ ) with

the phase variable  $\alpha = \beta$  for the case mentioned above. The minimizing orbits associated with distinct holes cannot self-intersect respectively; furthermore, they cannot intersect one another and others’ shifts. With such properties, they are termed *compatible* RO orbits [13].

A gap is generically composed of multiple openings whenever the potential has multiple “turning points” in a period. An *opening* is a certain amount of discontinuity associated with a turning point  $t_i$ , which, for example, can be a potential maximum near the anti-integrable limit [10] or a certain type of tip in the potential for the exactly solvable model discussed below (we expect that, in general, an opening can be attributed to every isolated concave part of the potential after TBA). The openings also come in orbits with a class of openings associated with each  $t_i$ . When more than one class of openings, say those associated with  $t_i$  and  $t_j$  with some  $i \neq j$ , merge to form a hole in the hull function; *i.e.*, each gap of the very hole consists of an opening associated with  $t_i$  and another with  $t_j$ , we say that the *resonance* occurs between these two classes of openings. The breaking of resonance occurs as the resonant gap split into more than one gap, each composed of at least one of the constituent openings of the original gap.

In this paper, our main goal is to demonstrate that, through studying exactly solvable models, whenever distinct openings in the hull function are in resonance, a non-recurrent rotationally ordered (NRO) configuration can be constructed. These NRO configurations can be thought of as *defects* imposed on the background of the recurrent RO (RRO) configurations. As it is well-known, defects are a very useful way of understanding phase transitions in FK models [1]. By adjusting the potential parameters, one can make the creation energy of these defects vanish, which signals a phase transition. Furthermore, with the employment of extended numbers [15] as elements in the phase parameter (defined later), the NRO configurations will be demonstrated to be depictable, similar to the RRO ones, by a hull function as in equation (5) and can be constructed as a limiting case of a sequence of RRO configurations.

The paper is organized as follows. In Section 2, the concept of “rotationally ordered” is reviewed to show that the existence of the two kinds of NRO orbits are generically allowed in the very concept. Extended numbers are naturally introduced in order to discern the NRO orbits from their background RRO ones. The well-known discommensuration in the commensurate case is discussed in an exactly solvable FK model in Section 3. The main purpose is to illustrate the concepts introduced in the previous sections, keeping in mind the conceptual similarities to the incommensurate case introduced in the following section, and to demonstrate the use of extended numbers in the hull function for the NRO configuration, which has not appeared in the literature before as far as we know. In Section 4, the incommensurate NRO configuration in another exactly solvable FK model is constructed by moving a certain atom, in an RRO configuration, to a neighboring potential well and depicted by using another type

of extended numbers as the phase parameter in the hull function. The phase transition mediated by the defects, in the NRO configuration, is discussed in Section 5. Here, we would like to emphasize the physical implication, while the mathematical details will be presented in another publication [17] which concentrates on solving the exactly solvable FK model.

## 2 Rotationally ordered orbits and extended numbers

In an invariant circle, the  $u$ -coordinates of the points are ordered according to their corresponding phase in the smooth hull functions and the mapping is *homeomorphic* and strictly increasing. Being RO is a remnant of this property after TBA. An RO orbit cannot self-intersect [10,12]. Consequently, for an RO configuration  $\mathbf{u}$  with irrational winding number  $\omega$ , there must be

$$\begin{cases} u_{n-s} + r > u_n, & \text{if } r > s\omega \\ u_{n-s} + r < u_n, & \text{if } r < s\omega \end{cases} \quad (7)$$

with  $r, s$  being integers and not both zero. When the winding number  $\omega = p/q$  is rational,  $r = s\omega$  with some  $r \neq 0$  is allowed, thus providing three choices to satisfy equation (4). The recurrent one is repetitious ( $u_{n+q} = u_n + p$ ) and without self-intersections except coincidence. Another choice is the one with a retarded elementary discommensuration (soliton) [4] where the winding number is, intuitively,  $(p/q)^-$  [5] and satisfies  $r(u_{n-s} + r - u_n) > 0$ , while  $r(u_{n-s} + r - u_n) < 0$  is observed by the third choice corresponding to the one with an advanced elementary discommensuration (anti-soliton) where the winding number is, intuitively,  $(p/q)^+$ . As we shall see below, the latter two choices of the winding number give rise to the NRO configurations in the commensurate case.

The  $(p/q)^-$  and  $(p/q)^+$  are the first kind of extended number, defined with respect to a dense subset in the interval  $[0, 1]$ , that we would like to include in the domain of the winding number. Let  $\mathcal{Q}$  be the rational numbers in  $[0, 1]$  and let  $\bar{\mathcal{Q}}$  denote all equivalent classes of strictly monotonic sequences of numbers in  $\mathcal{Q}$  with a limiting point. If the limiting point is not in  $\mathcal{Q}$ , the sequence can be identified with an irrational number. If the limiting point is  $p/q$ , an irreducible representation of an element in  $\mathcal{Q}$ , then we shall call  $(p/q)^-$  the (equivalent class of) strictly increasing sequences and  $(p/q)^+$  the (equivalent class of) strictly decreasing sequences in  $\bar{\mathcal{Q}}$  with this limiting point.

In the incommensurate case,  $\mathbf{u}$  can be depicted by a strictly increasing hull function such that  $u_n = f_\omega(n\omega + \alpha)$  with a certain phase variable  $\alpha$ . One can introduce another kind of extended number related to the partition of the  $x$ -axis according to the range in  $u = f_\omega(x)$ . Assume a period of potential can be divided into pieces according to some ‘‘turning points’’  $t_i$  with  $0 \leq t_i < 1$  (for example, in the anti-integrability limit or in the exactly solvable model discussed in Sect. 4) and

$$f_\omega(\beta_i - \epsilon) < t_i < f_\omega(\beta_i + \epsilon) \quad (8)$$

for some  $0 \leq \beta_i < 1$  and any arbitrarily small positive number  $\epsilon$ . If the hull function is smooth, one automatically has  $f_\omega(\beta_i) = t_i$ , but not so after TBA, where  $t_i$  can be inside the gap of  $f_\omega(x)$  at  $x = \beta_i$  with endpoints  $f_\omega^l(\beta_i)$  and  $f_\omega^r(\beta_i)$ . Suppose there are more than one turning point in a period of potential (which occurs in the FK model discussed in Sect. 4, but not in the one discussed in Sect. 3), say  $0 \leq t_j < t_i < 1$  with

$$f_\omega^l(\beta_j) < t_j < f_\omega^r(\beta_j) \leq f_\omega^l(\beta_i) < t_i < f_\omega^r(\beta_i) < 1 \quad (9)$$

for some  $0 \leq \beta_j < \beta_i < 1$ . Let us introduce  $n_{ij}(N)$  and  $n_{ji}(N)$  to be the integers  $n$  minimizing  $\text{Frac}[n\omega + \beta_j - \beta_i]$  and  $\text{Frac}[n\omega + \beta_i - \beta_j]$ , respectively, with  $-N \leq n \leq N$  for some positive integer  $N$ . If, as  $N \rightarrow \infty$ ,  $\text{Frac}[n_{ij}(N)\omega] = \text{Frac}[-n_{ji}(N)\omega]$  converges to  $\text{Frac}[n_{ij}\omega]$  with some finite value  $n_{ij}$ , then there are still three possibilities. One is  $n_{ij}(N) = -n_{ji}(N) = n_{ij}$  for all  $N \geq |n_{ij}|$ , which means that the openings associated with  $t_i$  and  $t_j$  are in resonance. For the other two choices, only one of  $n_{ij}(N)$  and  $-n_{ji}(N)$  equals  $n_{ij}$  for all  $N \geq |n_{ij}|$ , while the other diverges as  $N \rightarrow \infty$ . In both cases, the openings associated with  $t_i$  and  $t_j$  are adjacent to each other. Say,  $n_{ij}(N)$  diverges as  $N \rightarrow \infty$ , every point in the orbit denoted by  $f_\omega^r(\beta_j + n\omega)$  or  $f_\omega^l(\beta_i + n\omega)$  will have a *finite* opening associated with  $t_j$  on the left and another, with  $t_i$  on the right. As we shall see in the exactly solvable model below, such orbits correspond to the NRO configurations in the incommensurate case.

In fact, the limiting process of  $N \rightarrow \infty$ , as described above, must be conducted in taking the incommensurate case as a limit of commensurate cases [4]. More specifically, for a finite system, one can only consider commensurate cases. For the incommensurate case, one has to take the infinite large limit of the system size and then to take an irrational limit of the winding number  $\omega$ . This  $N$  is related to the denominator  $q$  of the rational winding number  $p/q$  in the limiting process approaching the irrational winding number as  $q \rightarrow \infty$ . More details will be given in [17].

For convenience, we would like to introduce the set  $\mathcal{S}_\omega \equiv \{\text{Frac}[n\omega] | n \in \mathcal{Z}\}$  of  $[0, 1]$ , with  $\omega$  in  $[0, 1]$ . The case with both  $n_{ij}(N)$  and  $n_{ji}(N)$  diverging as  $N \rightarrow \infty$  is equivalent to that with  $\beta_i - \beta_j \notin \mathcal{S}_\omega$ . To discern the three possibilities for  $\beta_i - \beta_j \in \mathcal{S}_\omega$ , we introduce the second kind of extended number. Again we denote  $\bar{\mathcal{S}}_\omega$  the set of equivalent classes of strictly monotonic sequences of elements in  $\mathcal{S}_\omega$ , which is a dense set in  $[0, 1]$  for irrational  $\omega$ , with a limiting point in  $[0, 1]$ . In case the limiting point  $\beta$  is in  $\mathcal{S}_\omega$ , we shall call  $\beta^-$  the (equivalent class of) strictly increasing sequences and  $\beta^+$  the (equivalent class of) strictly decreasing sequences in  $\bar{\mathcal{S}}_\omega$  with this limiting point.

With the employment of extended numbers in the hull function after TBA, it is crucial to note the order in taking the limits. Throughout this paper, *the righthand and lefthand side limits for the hull function will always be taken before the limits for the extended numbers.*

To scrutinize the *non-recurrent* configurations, one needs to consider a system with infinite size and with infinite number of atoms. The introduction of extended

numbers into the parameters of a hull function to depict a non-recurrent configuration indicates, on the one hand, that the hull function remains increasing so that the rotation order is preserved in the limiting procedure and, on the other hand, that an NRO configuration can always be constructed as a limiting case of RRO configurations when the system size approaches infinity.

### 3 Commensurate non-recurrent configurations

Now we would like to relate the construction of the minimum energy configurations with elementary discommensurations (commensurate NRO configurations), in a well-known exactly solvable model [2,16], to the resonance between openings. In this model, the potential  $V$  is a scalloped (piecewise parabola) function,

$$V(u) = \frac{1}{2} \left( \text{Frac}[u] - \frac{1}{2} \right)^2 \quad (10)$$

and there are tips in the potential at integer values of  $u$ . The force-balance equation is given by

$$u_{n+1} + u_{n-1} - (2 + \lambda)u_n = -\lambda b(u_n), \quad (11)$$

where  $b(u_n) \equiv \text{Int}[u_n] + 1/2$  gives the coordinate of the bottom of the potential branch that the  $n$ th atom resides in. The  $\{b(u_n)\}$  can be regarded as the coding sequence associated with  $\mathbf{u}$ . For an RO configuration  $\mathbf{u}$  satisfying equation (7),  $\{b(u_n)\}$  must also be RO in the sense that

$$\begin{aligned} b(u_n) - 1 &\leq b(u_{n-m}) + \text{Int}[m\omega]; \\ b(u_{n-m}) - \text{Int}[-m\omega] &\leq b(u_n) + 1. \end{aligned} \quad (12)$$

Note that both relations include equalities, no matter if  $\omega$  is rational or not, due to the fuzzy discrimination introduced by the discreteness of the code. Apparently,  $\mathbf{u}$  and  $\{b(u_n)\}$  must have the same winding number.

From equation (11), the stable configuration (where no atoms are allowed to sit on the tips of the potential, see [17,19] for details) is given by

$$u_n = d_0 \sum_{m=-\infty}^{\infty} e^{-|m|\chi} b(u_{n+m}) \quad (13)$$

with  $e^{-\chi} = (2 + \lambda - \sqrt{\lambda^2 + 4\lambda})/2$  and  $d_0 = \sqrt{\lambda/(\lambda + 4)}$ . For the solution to be self-consistent, there must be

$$|u_n - b(u_n)| < \frac{1}{2} \quad (14)$$

for each  $n$ . The ground state solution with winding number  $\omega$  can be depicted by equation (5) with

$$f_\omega(x) = d_0 \sum_{n=-\infty}^{\infty} e^{-|n|\chi} \tilde{b}(x + n\omega). \quad (15)$$

Note that  $\tilde{b}(x) = \text{Int}[x] + 1/2$ , termed the coding function, is an increasing function of the phase  $x$  and satisfies

$\tilde{b}(x+1) = \tilde{b}(x) + 1$ . The hull function is chosen to be right-continuous and  $f_\omega^l(0) < 0 \leq f_\omega^r(0) = f_\omega(0)$  is satisfied.

A commensurate ground state configuration with winding number  $\omega = p/q$  can accommodate elementary discommensurations which are either advanced (phase shift  $+1/q$ ) or retarded (phase shift  $-1/q$ ) [4]. A defective configuration with a fixed winding number can thus be interpreted as a distribution of these elementary discommensurations superimposed on a ground state configuration [9]. Now we would like to explicitly describe the minimum energy configuration with an elementary discommensuration using the local depiction property (see the Appendix).

Consider a minimum energy configuration with the winding number  $\omega = p/q$ . Suppose there is a retarded elementary discommensuration centered at  $u = \tilde{f}_\omega(p/2)$ , whose meaning will be evident after the explicit formula comes out. Here we use  $\tilde{f}_\omega(x)$  to denote  $[f_\omega^r(x) + f_\omega^l(x)]/2$ . Using the local depiction by the hull function with winding number  $\omega$ , the positions of the atoms can be described by

$$v_n = \begin{cases} f_\omega \left( \frac{np}{q} + \frac{1}{2q} \right) - \delta_- e^{n\chi}, & n \leq q; \\ f_\omega \left( \frac{np}{q} - \frac{1}{2q} \right) + \delta_+ e^{-n\chi}, & n \geq 0, \end{cases} \quad (16)$$

where  $\delta_-$  and  $\delta_+$  are both positive numbers and  $\delta_- + \delta_+ = d_q \equiv d_0(1 + e^{-q\chi})/(1 - e^{-q\chi})$ . The compatibility of these two formulas in the overlapping region yields

$$\delta_+ = \frac{d_0 + d_q}{2}; \quad \delta_- = \delta_+ e^{-q\chi}. \quad (17)$$

It is obvious that  $v_n \rightarrow f_\omega(\frac{np}{q} \pm \frac{1}{2q})$  as  $n \rightarrow \mp\infty$ . The largest deviation of the atomic position from its nearest allowable position of a ground state configuration with this  $\omega$  is given by  $\sqrt{\delta_+\delta_-}$ , occurring at  $v_{q/2} = \tilde{f}_\omega(p/2)$  for  $q$  even, or by  $\sqrt{\delta_+\delta_-}e^{-\chi/2}$ , occurring at  $v_{(q-1)/2}$  and  $v_{(q+1)/2}$  [symmetric with respect to  $u = \tilde{f}_\omega(p/2)$ ] for  $q$  odd. The elementary discommensuration is thus said to be centered at  $\tilde{f}_\omega(p/2)$ .

Now we can demonstrate below that  $v_n = f_\omega(n\omega)$  with  $\omega = (p/q)^-$ . For  $n \geq 0$  one has

$$\begin{aligned} & f_\omega(n\omega) - f_{p/q} \left( -\frac{1}{2q} + \frac{np}{q} \right) \\ &= d_0 \sum_{i=-\infty}^{\infty} e^{-|i|\chi} \left\{ \text{Int}[(n+i)\omega] - \text{Int} \left[ -\frac{1}{2q} + (n+i)\frac{p}{q} \right] \right\} \\ &= d_0 \sum_{i=-\infty}^{\infty} e^{-|i-n|\chi} \left\{ \text{Int}[i\omega] - \text{Int} \left[ -\frac{1}{2q} + i\frac{p}{q} \right] \right\} \\ &= d_0 \sum_{k=-\infty}^0 e^{-|n-kq|\chi} \\ &= \delta_+ e^{-n\chi}. \end{aligned}$$

Similar derivation yields  $f_\omega(n\omega) - f_{p/q}(\frac{1}{2q} + \frac{np}{q}) = -\delta_- e^{n\chi}$  for  $n \leq q$ . This proves  $v_n = f_\omega(n\omega)$  for  $\omega = (p/q)^-$ .

One can see that  $v_0 = d_0/2$ ,  $v_q = p - d_0/2$ , and no other atoms are within the  $d_0/2 + \delta_-(1 - e^{-qx})$  reach of their respective nearest tips. Note that in the minimizing orbits associated with  $\mathbf{v}$ , given by  $\{\text{Frac}[v_n]\}$  for all integers  $n$ , the two points  $v_0$  and  $v_q$  are neither repetitious nor accumulation points.  $\mathbf{v}$  is thus not recurrent. In the case with an advanced elementary discommensuration, similar relations with  $\omega = (p/q)^+$  can be derived straightforwardly.

It is obvious that the limit of  $f_\omega(n\omega)$  does not depend on the sequence we adopt for  $\omega = (p/q)^-$  as long as it satisfies our prescription. Though  $(p/q)^-$  and  $p/q$  have the same limiting value, the limits of the configurations depicted by them are, nevertheless, *distinct* (cannot to be made coincident by the shift operation). This is not so for  $\omega^-$  and  $\omega$  if  $\omega$  is irrational.

One can construct a representative sequence of  $(p/q)^-$  by choosing the rational number closest to  $p/q$  at each level of Farey fractions. In this construction, the configuration associated with  $(p/q)^-$  can be seen to be a soliton lattice in the limit of infinite lattice spacing [15].

It is interesting to note that all the RO stable configurations are automatically minimum energy configurations in the above mentioned FK model with a single well (or a single tip) in each period of potential (also note that there is only a uniquely determined  $\hat{b}(x)$  and the corresponding hull function for any given  $\omega$ ), while it is not necessarily the general case as we will see in the next example. For the potential with single tip in each period, there is only one class of gaps in the hull function. More specifically, from equation (15) one can see that there is a principal opening with width  $d_0$  at  $x = 0$  associated with the tip at  $u = 0$ . This principal opening carries a tower of secondary openings at  $x = \text{Frac}[n\omega]$  with widths  $d_0 e^{-|n|\omega}$  for all non-zero integers  $n$ . One should note that the total width of the openings is 1; hence, the openings in a period almost fill the interval  $[f_\omega^l(0), f_\omega^l(1)]$  and the allowed positions of atoms form either a discrete set or a cantorset.

In this model, resonance only occurs for rational winding numbers. That is, for irrational  $\omega$  all the openings do not resonate and there are infinitely many gaps of  $f_\omega(x)$  from  $x = 0$  to 1. While, for  $\omega = p/q$ , the openings merge into  $q$  gaps associated with  $x = i/q$  for  $0 \leq i < q$ . In the latter case, the width of the gap at  $x = 0$  is widened to  $d_q$  and the width of the gap at  $x = i/q$  is given by  $d_0 \sum_{n=-\infty}^{\infty} e^{-|nq+m|x}$  with some integer  $m$  satisfying  $\text{Frac}[mp/q] = i/q$ . Each gap consists of infinitely many openings in resonance. The process, as shown above, to construct the NRO configurations with winding number  $(p/q)^\pm$  from the repetitious one with winding number  $p/q$  can be understood as if the openings in the same gap for the latter case were forced to break their resonance and atoms were allowed to locate inside the gap. More specifically, for the configuration with  $\omega = p/q$  all the openings with the  $n$  satisfying  $n = i \pmod{q}$  for some  $0 \leq i < q$  merge to form a single gap; while for the one with  $\omega = (p/q)^-$  ( $\omega = (p/q)^+$ ), these openings are split apart and arranged consecutively in an descending (ascending) order with  $n$ . The limiting process in the definition of extended number  $(p/q)^-$  determines how these

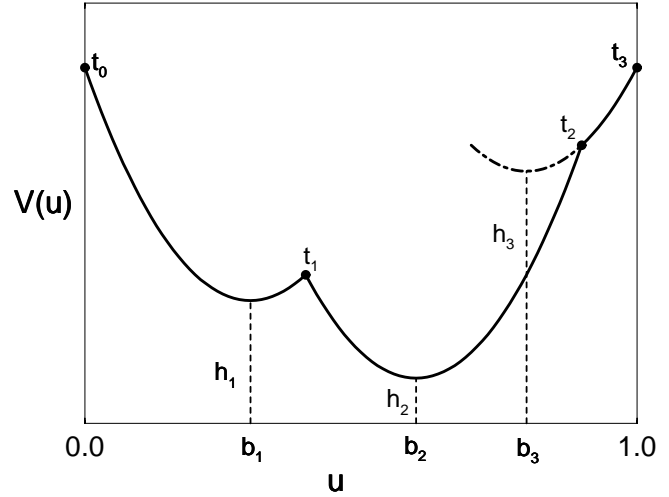


Fig. 1. Periodic potential  $V$  in equation (20) for  $d = 3$ .

openings are split in the breaking process. It is evident that such construction can only be conducted on the background with some openings in resonance.

#### 4 Incommensurate non-recurrent configurations

Next, we would like to turn to an extension of the Aubry model, where the potential has  $d$  subwells in a period. The study of such models will reveal some generic properties of the FK model after TBA. This model was first proposed by Griffiths *et al.* [8]. Some results were obtained in [19–21]; however, detailed analysis and understanding on the incommensurate NRO configurations are still lacking.

For there to be  $d$  pieces of parabolas in a period, the potential is given by

$$V(u) = \min_{1 \leq i \leq d} \{V_i(u)\} \quad (18)$$

for  $0 \leq u < 1$ , with

$$V_i(u) = \frac{1}{2}(u - b_i)^2 + h_i. \quad (19)$$

Here,  $h_i$  and  $b_i$ 's are independent parameters, arranged in the order  $b_1 < b_2 < \dots < b_d$ , with the constraint  $b_d < 1 + b_1$ . To take care of the fact that  $V(u)$  is periodic in  $u$  with period 1, one may set  $h_{d+i} = h_i$  and  $b_{d+i} = 1 + b_i$  for every integer  $i$  and equation (18) can be extended to

$$V(u) = \min_i \{V_i(u)\} \quad (20)$$

for any  $u$ . An example for  $d = 3$  is shown in Figure 1. Requiring  $V(u)$  to be continuous, the positions of the potential tips should be given by

$$t_i = \frac{b_i + b_{i+1}}{2} + \frac{\Delta h_i}{\Delta b_i}, \quad (21)$$

where  $\Delta h_i \equiv h_{i+1} - h_i$  and  $\Delta b_i \equiv b_{i+1} - b_i$ . In this expression,  $t_{d+i} = 1 + t_i$  is implied.  $t_i$ 's must satisfy

$$t_0 = 0 < t_1 < \dots < t_d = 1, \quad (22)$$

so that each branch of potential  $V_i(u)$  can be picked up for some  $u$  in equation (20). The condition,  $t_0 = 0$ , is chosen in order to be consistent with the definition in equation (18), which leads to the constraint  $h_1 + b_1^2/2 = h_0 + b_0^2/2$ . It should be noted that for  $t_{j-1} < u < t_j$ ,  $V_j(u)$  should be the one picked up to minimize  $V(u)$  in equation (20). This potential branch is named the  $j$ th subwell (or branch) and the collection of all those  $i$ th subwells with  $i = j \pmod{d}$  are named the  $j$ th type of subwells. The tips at the right ends of those subwells are called the  $j$ th tip and the  $j$ th type of tips, correspondingly.

The force-balance equation is again given by equation (11) but with the  $b(u_n)$  now given by  $b_i$ , if  $t_{i-1} < u_n < t_i$  (again,  $u_n$  won't sit on the tips in a stable configuration [17, 19]). The *formal* solution for a stable configuration is still given by equation (13).

Similar to the previous model, this one can have commensurate NRO configurations as well. However, we shall focus on the incommensurate NRO configurations which exist as a result of the resonance between openings associated with different types of tips, as shown below.

For an RRO configuration  $\mathbf{u}$  with irrational winding number  $\omega$ , the orbits  $\text{Frac}[u_n]$  keep the cyclic order as  $\text{Frac}[n\omega + \alpha]$  for some phase variable  $\alpha$ . Introduce the *phase parameter*  $\beta \equiv \{\beta_0 = 0 \leq \beta_1 \leq \dots \leq \beta_{d-1} \leq \beta_d = 1\}$  such that if, for every  $n$ ,  $\beta_{i-1} \leq \text{Frac}[n\omega + \alpha] < \beta_i$  holds for some  $0 < i < d$ , then  $t_{i-1} < \text{Frac}[u_n] < t_i$  is satisfied. We can define a right-continuous coding function  $\tilde{b}_\beta(x)$ , given by

$$\tilde{b}_\beta(x) = b_i, \quad \text{for } \beta_{i-1} \leq x < \beta_i, \quad (23)$$

which is increasing with  $\tilde{b}_\beta(x+1) = \tilde{b}_\beta(x) + 1$  and  $b(u_n) = \tilde{b}_\beta(n\omega + \alpha)$ . Then the hull function for  $\mathbf{u}$  can be derived straightforwardly and is given by [17, 21]

$$\begin{aligned} f_\omega(x) &= d_0 \sum_{n=-\infty}^{\infty} e^{-|n|x} \tilde{b}_\beta(n\omega + x) \\ &= d_0 \sum_{n=-\infty}^{\infty} e^{-|n|x} \text{Int}[x + n\omega] + d_0 \sum_{i=1}^d b_i \sum_{n=-\infty}^{\infty} e^{-|n|x} \\ &\quad \times (\text{Int}[x + n\omega - \beta_{i-1}] - \text{Int}[x + n\omega - \beta_i]) \\ &= 1 + b_j + d_0 \sum_{i=j}^{j+d-1} \Delta b_i \sum_{n=-\infty}^{\infty} e^{-|n|x} \text{Int}[x + n\omega - \beta_i] \end{aligned} \quad (24)$$

with any integer  $j$  and  $\omega \equiv (\omega, \beta)$ . The consistent condition is given by

$$f_\omega^l(\beta_i) < t_i < f_\omega^r(\beta_i) \quad (25)$$

for every  $i$ . The hull function depends only on  $\mathbf{b} \equiv \{b_0 < b_1 < \dots < b_{d-1} < 1 + b_0\}$  but not on  $\mathbf{t} \equiv \{0 = t_0 < t_1 <$

$\dots < t_{d-1} < t_d = 1\}$ .  $\mathbf{b}$  and  $\mathbf{t}$  exhaust all the  $2d-1$  degrees of freedom, except the uniform shifting in the potential level, in defining the  $d$ -subwell potential. Note that for a given  $\omega$ , there is a  $(d-1)$ -parameter family of RRO configurations, as compared to the uniqueness of that in the single-well model. Of course, most of them are not (global) minimum energy configurations. However, it is proved that, for any given  $\mathbf{b}$ , every RO configuration can be made to be a minimum energy one by a suitable choice of  $\mathbf{t}$  (in the form of Eq. (29) with details given in [17]). In the following we will see how the extra parameters  $\beta$  engender the possibilities of resonance between openings associated with different types of tips.

It is obvious from the hull function that there is a principal opening of width  $d_0 \Delta b_i$  associated with each  $x = \beta_i$ , or the tip  $t_i$ , for  $0 \leq i < d$  [22]. Each principal opening, say the  $i$ th one, carries a tower of secondary openings occurring at  $x = \text{Frac}[\beta_i + n\omega]$  with widths  $d_0 \Delta b_i e^{-|n|x}$  for all non-zero integers  $n$ . The sum of the widths of all the  $i$ th principal and secondary openings is  $\Delta b_i$  and  $\sum_{j=1}^d \Delta b_j = 1$ . Again, the allowed positions of the atoms form a cantor set in the incommensurate case.

When  $\beta_i - \beta_j \in \mathcal{S}_\omega$ , as defined above, for some  $0 \leq j < i < d$ , we say that they are *in resonance*. More specifically, if  $\beta_i = \beta_j + \text{Frac}[n_{ij}\omega]$ , the width of principal gap around  $t_i$  becomes  $d_0 \Delta b_i + d_0 \Delta b_j e^{-|n_{ij}|x}$  and the widths of the secondary gaps become  $d_0 \Delta b_i e^{-|n|x} + d_0 \Delta b_j e^{-|n+n_{ij}|x}$  for all  $n$ . Two classes of openings associated with  $\beta_i$  and  $\beta_j$  merge to form a single class of gaps. The resonance condition (termed ‘‘sub-commensurate condition’’ in [23]) is an equivalent relation which divides  $\{\beta_0 = 0, \beta_1, \dots, \beta_{d-1}\}$  into several subsets of equivalent  $\beta_i$ 's.

Now consider an incommensurate RRO configuration  $\mathbf{u}$  given by  $u_n = f_\omega(n\omega)$  with  $\beta_j = \text{Frac}[n_j\omega] \in \mathcal{S}_\omega$  for every  $0 \leq j < d$ . The  $n_j$ th atom is the one minimizing  $\text{Frac}[u_n - t_j]$  for each  $j$ . One can move the  $n_i$ th atom of  $\mathbf{u}$  across the nearest tip at its lefthand side (one of the  $i$ th type). After the configuration being stabilized (assume no more atoms move across a tip in this process which can always be achieved by proper choices of the parameters in the potential [17]), the resultant configuration, denoted by  $\mathbf{v}$ , is given by  $v_n = u_n - d_0 \Delta b_i e^{-|n-n_i|x}$  and one has  $u'_n < v_n < u_n$  for every  $n$  with  $u'_n = f_\omega^l(n\omega)$ . It is easy to check that the configuration  $\mathbf{v}$  is still RO and is *compatible* (has no crossing) with  $\mathbf{u}$  as well as  $\mathbf{u}'$ . However,  $\mathbf{v}$  is *not recurrent* because a section, with the  $m$ th atom located in one of the 1st type of subwells, say the  $(kd+1)$ th subwell, and the  $(m+n_i)$ th atom located in the  $(kd+i+\text{Int}[n_i\omega])$ th subwell, can only be found for  $m = k = 0$ , but not elsewhere. Some comments on the emergence of the incommensurate NRO configuration  $\mathbf{v}$  will be made further on.

Let  $\omega'$  denote  $\langle \omega, \beta_0, \dots, \beta_{i-1}, \beta_i^+, \beta_{i+1}, \dots, \beta_{d-1} \rangle$ . It is straightforward to show that

$$\begin{aligned} f_{\omega'}(n\omega) &= f_\omega(n\omega) + d_0 \Delta b_i \sum_{m=-\infty}^{\infty} e^{-|m|x} \\ &\quad \times (\text{Int}[(n+m)\omega - \beta_i^+] - \text{Int}[(n+m)\omega - \beta_i]) \\ &= u_n - d_0 \Delta b_i e^{-|n-n_i|x}, \end{aligned} \quad (26)$$

which gives  $v_n = f_{\omega'}(n\omega)$ .

Since all the  $d$  classes of openings, each associated with a tip  $t_j$  with  $0 \leq j < d$ , are in resonance for the configuration  $\mathbf{u}$ , there is only one hole. In particular, at  $x = \text{Frac}[n\omega]$ , the width of the gap is given by  $d_0 \sum_{j=0}^{d-1} \Delta b_j e^{-|n-n_j|x}$ , which is the very gap between  $u_n$  and  $u'_n$ . The atom  $v_n$  is now located inside the gap. There is no longer an atom closest, from above, to the  $i$ th type of tips although there are still atoms closest to the  $j$ th type of tips for all  $j \neq i$ . We can construct  $\beta_i^+$  by choosing a sequence of integers  $\{n_{ik}|k=1,2,\dots\}$  such that  $\text{Frac}[n_{ik}\omega] > \text{Frac}[n_{i,k+1}\omega]$  and  $\lim_{k \rightarrow \infty} \text{Frac}[n_{ik}\omega] = \text{Frac}[n_i\omega]$ . Clearly  $\lim_{k \rightarrow \infty} |n_{ik}| = \infty$  so that the atom closest to the  $i$ th type of tips “moves off” to spatial infinity. The restriction of the elements, in the sequence  $\beta^+$ , to belong to  $\mathcal{S}_\omega$  would facilitate the construction of the NRO configuration as a limit of RRO ones.

In the  $\mathbf{v}$  configuration, the atom originally at  $u_{n_j}$ ,  $j \neq i$ , moves from the upper end of the gap, of  $f_\omega(x)$  at  $x = \beta_i$ , to  $v_{n_j}$ , which is inside the very gap. It is clear that  $|\text{Frac}[v_n] - \text{Frac}[v_{n_j}]| > \min(\Delta v_{n_j}, \Delta_j - \Delta v_{n_j})$  with  $\Delta v_{n_j} \equiv u_{n_j} - v_{n_j}$  and  $\Delta_j \equiv u_{n_j} - u'_{n_j}$ , for any  $n$  other than  $n_j$ , also indicating that the  $\mathbf{v}$  configuration is non-recurrent. Besides, every gap of the RRO configuration, say the one between  $u_n$  and  $u'_n$ , is divided into two by the  $v_n$ . The one on the right, *i.e.*, between  $u_n$  and  $v_n$ , is the principal or a secondary opening associate with  $t_i$ , while the other is the gap consisted of the  $d-1$  openings, each associated with one of the  $t_j$  with  $j \neq i$ . Namely, the NRO configuration is again constructed by breaking the resonance. One should also note that  $\lim_{n \rightarrow \pm\infty} u_n - u'_n = \lim_{n \rightarrow \pm\infty} v_n - u_n = 0$ . The orbit of  $\mathbf{v}$  is *homoclinic* to that of  $\mathbf{u}$  and the cantorus associated with  $\mathbf{v}$  has a two-hole structure [17].

Since the  $n_j$ th atom for  $j \neq i$  is still the atom closest, from above, to the  $j$ th type of tips in the defect configuration, we can move it over the tip to its left neighboring well resulting in a new NRO configuration with

$$w_n = u_n - d_0 \Delta b_i e^{-|n-n_i|x} - d_0 \Delta b_j e^{-|n-n_j|x} = f_{\omega''}(n\omega) \quad (27)$$

and

$$\omega'' = \langle \omega, \beta_0, \dots, \beta_{i-1}, \beta_i^+, \beta_{i+1}, \dots, \beta_{j-1}, \beta_j^+, \beta_{j+1}, \dots, \beta_{d-1} \rangle.$$

It should be obvious how to generalize this construction of the incommensurate defects.

In general, the resonance conditions divide  $\{\beta_0, \beta_1, \dots, \beta_{d-1}\}$  into  $m$  subsets of equivalent  $\beta_i$ 's. There are  $m$  distinct holes in the cantori. Correspondingly, there exist  $m$  distinct type of orbits. The incommensurate defects can be constructed for each of the  $m$  subsets of the equivalent  $\beta_i$ 's. Let  $\{\beta_{i_1}, \dots, \beta_{i_k}\}$  be such a subset. An NRO configuration can be constructed by allowing one or more of the differences  $(\beta_{i_j} - \beta_{i_1}) \in \mathcal{S}_\omega$  to become extended numbers in  $\mathcal{S}_\omega$ . In practice, this is achieved by choosing the phase variable  $\alpha$  in equation (5)

to equal  $\beta_{i_1}$  first. The NRO configurations are then obtained as described for the case of  $m=1$ .

It should be clear now how the NRO orbits arise by the breaking of resonance. After TBA, the hull function becomes discontinuous with a system of gaps. Some of the gaps are composed of multiple openings when resonance occurs. For an NRO orbit, a generic point lies inside a gap so that there are openings of finite widths at its two sides. In contrast, a generic point of an RRO orbit lies at the end of a gap with a finite opening on one side and an infinitesimal opening on the other side. An NRO configuration can be constructed from the corresponding background RRO one by adding or removing an atom, as in the commensurate case, thus forcing atoms into the gaps as the system relaxes. The resulting discommensuration carries a particle number of  $1/p$  for  $\omega = p/q$  and is a typical example of topological defects. Another way of constructing NRO configuration from its background RRO one is to move one atom closest to a certain “turning point”  $t_i$  of the potential to the other side of  $t_i$ , as in the incommensurate case, again forcing atoms into the gaps. In so doing, there no longer exists an atom closest to  $t_i$  (from the side where the atom was moved), at finite spatial extent of the system, in the resulting NRO configuration. The resulting defect does not carry particle number and is non-topological.

## 5 The defect-mediated phase transition

The defect-mediated commensurate-incommensurate phase transition by the discommensurations was described in [1]. It is instructive to review some of the previous results which bear a certain similarity with the case of interests. The phase diagram ( $\omega$  vs. the tensile force  $\sigma$ ) of the model discussed in Section 3 was a complete Devil's staircase, as explicitly derived in [16]. In the phase diagram, each rational (winding number) carries a plateau with finite width. At the end point of each plateau, the recurrent ground state configuration has the enthalpy degenerate with that of a non-recurrent minimum energy one with an elementary discommensuration. Note that the creation enthalpy of a retarded (advanced) discommensuration increases (decreases) with  $\sigma$ . Beyond the value of  $\sigma_c$  at which the corresponding creation enthalpy vanishes, there is a competition between two effects: the negative creation enthalpy of a discommensuration which favors the formation of as many of them as possible, and the repulsive interaction between them, favoring a density of discommensurations as low as possible. The compromise between both effects determine the new ground state structure (with winding number close to that for the plateau) close to  $\sigma_c$ .

Now let us turn to the defects resulting in the incommensurate NRO configurations. As  $t_i$ 's are varied in the region in  $\mathbf{t}$  space, where the ground state configuration is locked to  $\beta_i = \text{Frac}[n_i\omega]$  for  $i = 1, \dots, d-1$  [17,19,21], boundaries consisting of pieces of hypersurfaces of dimensions lower than  $d-1$  will be reached. These boundaries are determined by the conditions that the energy of a certain defect configuration, as constructed

in the last section, equals the energy of its recurrent background ground state configuration. In particular, taking the  $\mathbf{u}$  and  $\mathbf{v}$  configurations, discussed above, as the example, one has

$$\begin{aligned} H(\mathbf{v}) - H(\mathbf{u}) &= \\ &\sum_n \left\{ \frac{1}{2} (v_{n+1} - v_n)^2 + \frac{\lambda}{2} [v_n - b(u_n) + \delta_{n,n_i} (b_i - b_{i+1})]^2 \right\} \\ &- \sum_n \left\{ \frac{1}{2} (u_{n+1} - u_n)^2 + \frac{\lambda}{2} [u_n - b(u_n)]^2 \right\} + \lambda (h_i - h_{i+1}) \\ &= \lambda \Delta b_i \left( u_{n_i} - t_i - \frac{d_0}{2} \Delta b_i \right). \end{aligned} \quad (28)$$

It follows that for the  $\mathbf{u}$  and  $\mathbf{v}$  configurations to be degenerate, the condition

$$t_i = \frac{f_\omega(\beta_i) + f_{\omega'}(\beta_i)}{2} \quad (29)$$

must be fulfilled, which gives the equation for the boundary. At these boundaries (hypersurfaces with dimensionality smaller than  $d - 1$ ), non-recurrent (globally) minimizing orbits, like  $\mathbf{v}$ , are allowed.

As  $\mathbf{t}$  is moved beyond the boundary, there is competition between two effects. The atoms with positions (in the orbit) arbitrarily close to  $\text{Frac}[u_{n_i}]$  are energetically favorable to move across their neighboring tips of type  $t_i$ , which favors the formation of as many of them (the defects) as possible with the consequent shift of  $\beta_i$ . On the other hand, there is the repulsive interaction between the defects. Since, to keep the orbit minimum energy, the orbit must be rotationally ordered, thus the defects energetically prefer to be distributed uniformly on the system of infinite size. That is to say, they will repel one another to minimize the energy. The effect favors a density of such defects as low as possible. The compromise between both effects determine a new ground state structure (with a different but close  $\beta_i$ ).

The types of boundaries are classified according to the types of defect configurations [17]. At the boundaries, the single hole is just about to break into two or more holes. For more tips in resonance, one may construct more distinct (unable to be made coincident by the shift operation) compatible RO configurations through the appropriate movements of atoms across tips, each equivalent to breaking one class of the resonance. All of the compatible RO configurations can become minimum energy configurations by a suitable choice of  $\mathbf{t}$  (Eq. (29) specifies the condition for only one atom moved across tips, while the general case is derived in [17]). They can be minimizing only when all of them are degenerate. Say, there are  $m$  of them, there would be  $m - 1$  conditions, like equation (29), to determine a  $(d - m)$ -dimensional hypersurface in the  $\mathbf{t}$  space. The system is locked in a finite  $(d - m)$ -dimensional region. The boundaries of the region, with dimensionality lower than  $d - m$ , are determined by the conditions that an additional type of incommensurate defect have the same energy as the recurrent background. For there to be  $d$  subwells in a period of potential, there are at most  $d - 1$  types

of NRO configurations for a given RRO background since there are  $d - 1$  independent  $\beta_i - \beta_j$  for  $0 \leq j < i < d$ .

## 6 Conclusion

While the incommensurate NRO configurations were known to exist, their properties and production mechanism were not clear. On the other hand, there were indications that the cantorus resulting from the breaking of an invariant curve can be composed of multiple holes (*i.e.*, classes of gaps). We pointed out that these two phenomena are closely related. Whenever the resonance conditions hold, a gap is composed of multiple openings and atoms can be moved from the end of a gap inside the gap resulting in an NRO configuration. The incommensurate defect so produced in general has higher energy per atom over the corresponding background RRO configuration which is a ground state. At critical value of the parameters in the potential, the defect configuration is degenerate with the ground state RRO configurations. A first order phase transition occurs and the gap is about to splitting into two or more gaps, revealing the multiple hole structure of the cantorus.

The existence of NRO configurations shows that for given winding number  $\omega$  and phase parameters  $\beta$ , there may be more than one increasing hull function. They can be distinguished by introducing the concept of extended numbers for  $\omega$  and  $\beta_i$ 's. The limiting procedure inherent in the definition of extended numbers indicates how the NRO configuration can be constructed as the limit of a sequence of RRO configurations.

Although a specific model was employed to demonstrate certain intrinsic properties of NRO configurations, we expect their relations to dynamical systems and to phase transitions are generic and worth further investigation.

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## Appendix

We would like to show an interesting property, termed *the local depiction*, enjoyed by the FK model with potential composed of parabolic branches with the same curvature  $\lambda$ . Assuming  $b(u)$  gives the coordinate of the bottom of the potential branch which  $u$  belongs to. For any two stable atomic configurations  $\mathbf{u}$  and  $\mathbf{v}$ , one has

$$u_{n+1} + u_{n-1} - 2u_n = \lambda [u_n - b(u_n)]$$

and

$$v_{n+1} + v_{n-1} - 2v_n = \lambda [v_n - b(v_n)].$$

After appropriate shift of the subscript  $n$  in  $v_n$ , one can manage to make  $b(u_n) = b(v_n)$  holds for all  $n$  respecting



$n_- < n < n_+$ . In this region one has

$$(u_{n+1} - v_{n+1}) + (u_{n-1} - v_{n-1}) = (2 + \lambda)(u_n - v_n).$$

Accordingly, there must be

$$u_n - v_n = \Delta_+ e^{n\chi} + \Delta_- e^{-n\chi} \quad (\text{A.1})$$

for  $n_- \leq n \leq n_+$  with the correlation length  $1/\chi$ .  $\Delta_+$  and  $\Delta_-$  are obtainable from  $u_n - v_n$  for any two distinct  $n$ 's in  $[n_-, n_+]$ . Therefore, the local depiction of  $\mathbf{v}$  using  $\mathbf{u}$ , accompanied by appropriate distortions with characteristic length  $1/\chi$ , is feasible for  $n_- \leq n \leq n_+$ . In particular, any stable atomic configuration  $\mathbf{u}$  can be depicted locally by a hull function  $f_\omega(x + n\omega)$ , accompanied by appropriate distortions, as long as  $b(u_n) = \tilde{b}(x + n\omega)$  holds in some  $n$  with suitably chosen  $\omega$  and  $x$ . Practically point by point calculation using equation (11) is no longer necessary in tracing an orbit of the twist map since the positions of some distant points are thus within easy reach using the above relations.

If any two neighboring atomic positions,  $u_n$  and  $u_{n+1}$ , can be depicted by some hull function with zero  $\Delta_+$  ( $\Delta_-$ ) and the distortion at the right (left) one doesn't cause that atom to move to another potential well, the local depiction can be extended to a global depiction. Namely, all the atomic positions to their right (left) can be depicted by the very hull function accompanied by the distortion described by  $\Delta_-$  ( $\Delta_+$ ), which means that  $u_n$  approaches the atomic position characterized by this hull function as  $n \rightarrow \infty$  ( $-\infty$ ). In terms of dynamic systems, the orbit is *asymptotically (quasi-)periodic* and not chaotic for the forward (backward) iteration. In addition, if one can find two hull functions  $f_{\omega_1}$  and  $f_{\omega_2}$ , respectively, with zero  $\Delta_+$  and  $\Delta_-$  to describe an atomic configuration  $\mathbf{u}$  to its right and left ends, then the depiction of  $\mathbf{u}$  can be covered by segments of a finite number of hull functions with accompanying distortions (an explicit example can be found in equation (16) where an elementary discommensuration is described). Clearly, this orbit is heteroclinic to the two depicted by  $f_{\omega_1}$  and  $f_{\omega_2}$ . However, different appearances of this property for other kinds of potential and their accompanying twist maps should be expected.

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22. Contrary to the statement proposed in [10], each type of tip in our model carries a class of openings in the cantorus, no matter if the tip is a potential maximum or not (for example, see the tip  $t_2$  in Fig. 1). Naturally, we conjecture that each section of potential with  $V'''(u) < 0$ , separated by sections with  $V'''(u) \geq 0$ , could carry a class of openings by itself. To identify the elements which carry classes of openings by their own is relevant to the identification of the coding sets needed to describe the orbits symbolically.
23. S. Aubry, F. Axel, F. Vallet, J. Phys. C **18**, 753 (1985).