

## Exactly Solved Frenkel-Kontorova Model — Almost Everywhere Concave Potential

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We solved the Frenkel-Kontorova model with the potential  $V(u) = -\lambda(u - \text{Int}[u] - 1/2)^2/2$  exactly. The minimum energy configurations and recurrent configurations with fixed winding number are completely characterized. The average energy per atom of different configurations are explicitly calculated, which is used to determine the ground state configuration with a given winding number. The evolution of the ground state configurations is shown to be dictated by the Farey fractions.

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### I. Introduction

Periodic modulated structures are quite common in condensed matter physics. In general there is a tendency for the periodicity to lock into values which are commensurable with the lattice constant [1]. As external parameters are varied, the system may pass through several commensurate phases with or without incommensurate phases between them.

Generically the periodicity may take every single commensurable value in an interval. As the rational numbers are everywhere dense, any two steps in the plot of the function showing the periodicity versus the control parameter are thus always separated by infinitely many steps. Such a structure is called the devil's staircase [2]. In particular, if the commensurate phases fill up the whole phase diagram, the staircase is said to be complete.

The Frenkel-Kontorova (FK) model provides such an example of commensurate-incommensurate transition. This model describes a linear chain of coupled atoms in an external periodic potential. The enthalpy [3] of the system has the form

$$H(\{u_n\}) = \sum_n \left[ \frac{1}{2}(u_{n+1} - u_n)^2 + \lambda V(u_n) - \sigma(u_{n+1} - u_n) \right], \quad (1.1)$$

where  $u_n$  is the position of the  $n$ th atom and  $\sigma$  is a tensile force which allows the atomic distance between neighboring atoms to be changed continuously in the absence of the periodic potential. The periodic potential  $\lambda V(u)$  has amplitude  $\lambda$  and period 1, which can be set to 1 with suitable choice of the length scale. For a stationary configuration one has  $\partial H / \partial u_n = 0$  and thus

$$u_{n+1} - 2u_n + u_{n-1} = \lambda V'(u_n), \quad (1.2)$$

which can be formulated as a two-dimensional area-preserving circle map [4]. In this language,  $\lambda$  can be looked upon as a measure of the nonlinearity and a stationary configuration in the FK model corresponds to an orbit in the circle map. One notes that in Eq. (1.2) the tensile force term drops out and is irrelevant in determining the stationary configuration. Hence, Eq. (1.1) with the tensile force term discarded would be defined as the system energy.

For a smooth potential  $V(u)$ , Aubry [5,6] defines a minimum-energy configuration  $\{u_n\}$  as the one in which  $H$  cannot be decreased by altering a finite number of  $u_n$ . Under this circumstance, there is a well-defined winding number (not in our case)

$$\omega = \lim_{N, N' \rightarrow \infty} \frac{u_N - u_{-N'}}{N + N'}. \quad (1.3)$$

which is also the mean atomic distance. A ground state is by definition a recurrent minimum-energy configuration, whose atomic positions can be characterized by [5,6]

$$u_n = f_\omega(n\omega + \alpha). \quad (1.4)$$

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

$$f_\omega(x + 1) = f_\omega(x) + 1, \quad (1.5)$$

i.e.,  $f_\omega(x) - x$  is a periodic function with the period of the potential and  $\alpha$  is a phase variable which determines the relative position of the atomic chain with respect to the periodic potential. In this case, a ground state configuration with rational  $\omega = p/q$  consists of "molecules" that are composed of  $q$  particles and  $p$  wells. Here, we would like to emphasize that a ground state configuration must be a minimum energy configuration and a minimum energy configuration must be a stationary configuration.

Aubry first studied an interesting model with piecewise, almost everywhere convex, parabolic potential and obtained the ground state configurations as well as the phase diagram rigorously [4,7,8]. The potential of this model has cusps at the potential maxima. In a given ground state configuration, there can be no atom in the close vicinity of the cusps [9,10]. This property greatly facilitates the analytical analysis. If the potential well is inverted so as to become almost everywhere concave, the cusps will be located at the bottom of the potential wells. The effect resulting from the possibility of atoms being pinned at those cusps, as we shall see, is drastic. Specifically, the ground state configurations are highly degenerate and, for a given  $\lambda$ , only a finite set of rational numbers can be the winding number of a lowest enthalpy configuration. The plot of the function of the periodicity versus the external parameter (in this case, the tensile force) is thus a harmless staircase rather than a devil's staircase.

In this paper, we'd like to focus on the case with cusps at the bottom and derive the exact solution of the ground state configuration. The physical implications of these results have been published elsewhere [11,12], while all the mathematical details in deriving the ground state configurations and calculating the average energy per atom of these systems will be provided below.

The paper is organized as follows. In Sec. II, we define the model and derive some properties specific to the stationary configurations of this model. The explicit form of the atomic positions for sections and recurrent configurations are given in Sec. III. In Sec. IV, expressions for the average energy per atom of all the configurations considered in Sec. III are derived. Using these results, we establish the ground state configurations of this model in Sec. V.

## II. The model

In the exactly solvable model the potential  $V$  is a scalloped (piecewise parabola) function,

$$V(u) = -\frac{1}{2} \left( u - \text{Int}[u] - \frac{1}{2} \right)^2, \quad (2.1)$$

where  $\text{Int}[u]$  is the largest integer not greater than  $u$ . The average energy per atom in the ground state configuration is given by

$$\Psi_e(\omega) \equiv \left\langle \frac{1}{2} (u_{n+1} - u_n)^2 \right\rangle + \lambda \left\langle V(u_n) \right\rangle \quad (2.2)$$

where  $\langle \dots \rangle$  denotes the average over the whole system.

The derivative of the potential  $V$  has discontinuities at each integer. These discontinuities, unlike the case where they are on the maxima of the potential [9,10], have conspicuous effect on the minimum energy configurations. Firstly, they locate at the bottom of the potential wells and the atoms have a tendency to approach them to lower the energy of the system. For example, as  $\lambda \rightarrow \infty$ , one expects that all of the atoms should sit at the cusps. In fact, as we shall see in a moment, for any finite  $\lambda$ , there are always atoms sitting at the cusps for any minimum energy configuration. Secondly, the atoms located at the cusps can sustain forces with a magnitude smaller than  $\lambda/2$ ; namely, these atoms need not satisfy Eq. (1.2), but obey

$$-\frac{\lambda}{2} \leq u_{n+1} + u_{n-1} - 2u_n \leq \frac{\lambda}{2} \quad (2.3)$$

for the  $n$ -th atom that is pinned. As shown below, this flexibility in assigning forces for the pinned atoms results in a large number of degenerate ground state configurations.

From Eq. (2.3) we know that the stationary configurations need not be symmetrical with respect to an atom pinned at the cusps. A pinned atom thus allows us to join two different stationary configurations, each of which has at least one atom located at the cusps. Therefore, for a configuration with  $u_0 = 0$ ,  $u_q = p$  and none of the in-between atoms pinned at the cusps, we shall say that the  $q$  atoms,  $\{u_0, u_1, \dots, u_{q-1}\}$  form a "  $p/q$ -section" .

Consider a stationary configuration with a segment of  $q-1$  consecutive atoms,  $\{u_1, u_2, \dots, u_{q-1}\}$ , none pinned at the cusps. One can study the phonon spectrum of this segment with all the other atoms fixed. The energy of this system is given by

$$H(\{u'_n\}) = H(\{u_n\}) + \sum_{k=1}^{q-1} \frac{\partial H(\{u_n\})}{\partial u_k} \delta u_k + \sum_{k,j=1}^{q-1} \frac{\partial^2 H(\{u_n\})}{\partial u_k \partial u_j} \delta u_k \delta u_j, \quad (2.4)$$

where  $\delta u_k \equiv u'_k - u_k$  is the displacement of the  $k$ -th atom. For a stationary configuration, the second term in the righthand side vanishes. Denoting the column vector  $\delta \mathbf{u} \equiv \text{col}(\delta u_1, \delta u_2, \dots, \delta u_{q-1})$ , the third term can be expressed as a quadratic form,  $(\delta \mathbf{u})^T \mathbf{M}(\delta \mathbf{u})$ , where  $\mathbf{M}$  is a  $(q-1) \times (q-1)$  matrix, given by

$$\mathbf{M}(i, j) = \begin{cases} 2 - \lambda, & \text{if } i = j; \\ -1, & \text{if } i = j \pm 1; \\ 0, & \text{otherwise.} \end{cases} \quad (2.5)$$

One can derive that

$$\det \mathbf{M} = \frac{\sin q\chi}{\sin \chi} \quad (2.6)$$

with  $\chi = \arccos(1 - X/2)$ ,  $0 \leq \lambda \leq 4$ .  $\chi$  is a monotonically increasing function of  $\lambda$  and can be used, instead of  $\lambda$ , as the parameter characterizing the nonlinearity. As  $\lambda$  increases from 0,  $\mathbf{M}$  is positive definite and these  $q-1$  atoms are in a stable position until  $\chi = \chi_q \equiv \pi/q$ . At this point, there appears a zero frequency phonon mode with  $\delta u_k \propto \sin k\chi$ . When  $\chi > \chi_q$ , there is a phonon mode with imaginary frequency; i.e., the segment becomes unstable. Therefore, we have the following theorem.

**Theorem 1.** *For a stationary configuration of the FK model determined by Eqs. (1.2), (2.1), and (2.3), there cannot be consecutive  $q-1$  atoms, none pinned at the cusps, in a minimum energy configuration for  $\chi > \chi_q$ .*

This theorem shows that for given  $\chi$ , minimum energy configuration must be composed of sections.

For the convenience of subsequent discussions, let us introduce the notion of the "Farey fractions" [13], which is defined as the collection of all irreducible fractions in  $[0, 1]$ , arranged in an ascending order. The " $q$ -th row" of Farey fractions is defined as the Farey fractions where irreducible fractions with denominator larger than  $q$  are truncated. In a  $q_c$ -th row of Farey fractions, an irreducible fraction  $w = p/q$  has two nearest neighbors,  $\omega_1 = p_1/q_1$  and  $\omega_2 = p_2/q_2$ , such that

$$\kappa p = p_1 + p_2, \quad \kappa q = q_1 + q_2, \quad \omega_1 < \omega < \omega_2 \quad (2.7)$$

for some positive integer  $\kappa$  and

$$p q_1 = p_1 q + 1, \quad p_2 q = p q_2 + 1, \quad p_2 q_1 = p_1 q_2 + \kappa. \quad (2.8)$$

It should be noted that for given  $p/q$ , the values of  $p_1/q_1, p_2/q_2$ , and  $\kappa$  are dependent on  $q_c$ . For instance, assume  $p/q = 3/5$ , then  $p_1/q_1 = 1/2, p_2/q_2 = 2/3$ , and  $\kappa = 1$  for  $q_c = 6$ ; however,  $p_1/q_1 = 4/7, p_2/q_2 = 5/8$ , and  $\kappa = 3$  for  $q_c = 9$ . When  $q_c = q$ ,  $\kappa$  is 1 and the corresponding  $p_i, q_i, \omega_i$  are denoted by  $p_i^0, q_i^0, \omega_i^0$ , respectively.

From Theorem 1, we know that for  $\chi_{q_c+1} < \chi \leq \chi_{q_c}$ , we only need to consider those  $w$ -sections with  $w$  in the  $q_c$ -th row of the Farey fractions in searching for the minimum energy configurations. For a section beginning at  $u_0 = 0$ , a formal solution consistent with Eqs. (1.2), (2.1), and (2.3) is given by

$$u_0 = 0, \quad (2.9)$$

$$u_1 = s_0 \sin \chi, \quad (2.10)$$

$$u_2 = s_0 \sin 2\chi + l_1 \sin \chi, \quad (2.11)$$

$$u_3 = s_0 \sin 3\chi + l_1 \sin 2\chi + l_2 \sin \chi, \quad (2.12)$$

$$\vdots$$

$$u_q = s_0 \sin q\chi + \sum_{k=1}^{q-1} l_k \sin(q-k)\chi, \quad (2.13)$$

where  $s_0$  is a parameter that can be determined by  $u_1$  and, for  $1 \leq k \leq q-1$ ,  $l_k \equiv \gamma M_k$  with  $\gamma \equiv \lambda / \sin \chi = 2 \tan(\chi/2)$  and  $M_k \equiv \text{Int}[u_k] + 1/2$ , if the  $k$ -th atom is not pinned and  $l_k \in [\gamma M_{k-1}, \gamma M_k]$ , if the  $k$ -th atom is pinned. Let us consider Eq. (2.11) first. If the coefficients,  $\sin 2\chi$  and  $\sin \chi$ , are positive,  $s_0$  (or  $u_1$ ) and  $l_1$  can be regarded as increasing functions of  $u_2$ , as shown in Fig. 1. Namely, if  $u_1$  is pinned, then  $s_0$  is a constant and  $l_1$  increases with  $u_2$ ; on the other hand, if  $u_1$  is not pinned, then  $l_1$  is a constant and  $s_0$  increases with  $u_2$ . Any combination of  $s_0$  and  $l_1$  with positive coefficients is a monotonically increasing function of  $u_2$ .

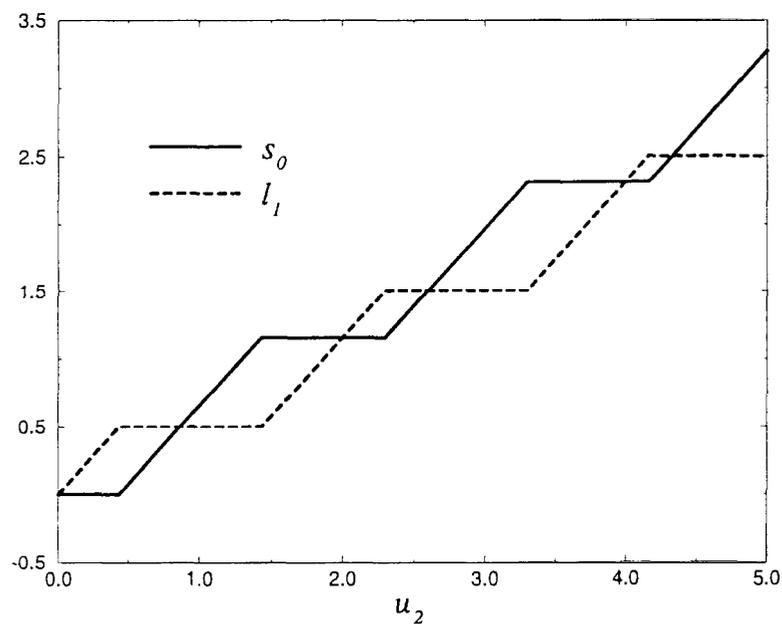


FIG. 1.  $s_0$   $l_1$   $u_2$   $\lambda = 1$

Now consider Eq. (2.12). If  $\sin 3\chi$  is still positive, then the sum of the first two terms in the righthand side is a monotonically increasing function of  $u_2$ . With the same argument as above,  $u_2$  and  $l_2$  can be regarded as increasing functions of  $u_3$ . If  $u_2$  is pinned, then  $u_2$  is a constant, so are  $s_0$  and  $l_1$ , and  $l_2$  increases with  $u_3$ ; on the other hand, if  $u_2$  is not pinned, then  $l_2$  is a constant and  $u_1$  increases with  $u_2$ , accompanied with the increase in either  $s_0$  or  $l_1$ . Therefore,  $s_0$  and  $l_1$  are also increasing functions of  $u_3$  and any combination of  $s_0$ ,  $l_1$ , and  $l_2$  with positive coefficients is a monotonically increasing function of  $u_3$ .

Similar arguments can be carried on up to  $u_q$  if all the coefficients of  $l_i$  are positive. Therefore, we have the following theorem.

**Theorem 2.** In a stationary configuration of the FK model determined by Eqs. (1.2), (2.1), and (2.3) with  $u_0 = 0$  and  $\chi < \chi_q$ ,  $u_r$  is an increasing function of  $u_s$  for  $0 < r < s \leq q$ .

An obvious consequence of this theorem is as follows.

**Corollary 1.** The  $p/q$ -sections are uniquely determined for  $\chi < \chi_q$ .

For reducible  $p/q$ , we can find some positive integer  $\kappa$  so that  $p = \kappa p_0$  and  $q = \kappa q_0$  with  $p_0/q_0$  irreducible.  $\kappa p_0/q_0$ -sections are able to coalesce into a segment with  $u_0 = 0$  and  $u_q = p$ . For  $\chi < \chi_q$ , this is the only way to satisfy these two boundary conditions and the equation of motion, but this segment cannot be regarded as a "section" since some of the in-between atoms are pinned. Therefore, in the remaining part of this paper, all the fractions mentioned are assumed to be irreducible.

Moreover, if, in addition to  $u_0 = 0$ , there are two more atoms,  $u_i$  and  $u_j$ , being pinned with  $0 < i < j \leq q$ , we can find another stationary configuration,  $v_n = u_j - u_{j-n}$  with  $0 \leq n \leq j$ , satisfying  $v_0 = 0$ ,  $v_{j-i} = u_j - u_i$ , and  $v_j = u_j$ . From Theorem 2, we must have  $j = 2i$  and  $u_j = 2u_i$ , which leads to the following corollary.

**Corollary 2.** Two different sections,  $p_1/q_1$  and  $p_2/q_2$ , cannot be connected in a stationary configuration for  $\chi < \chi_{q_1+q_2}$ .

Consider a section described by  $v_n = p - u_{q-n}$  for  $0 \leq n \leq q$ , where  $\{u_n | n = 0, 1, \dots, q\}$  denotes a  $p/q$ -section with  $u_0 = 0$  and  $u_q = p$ . As  $\{v_n | n = 0, 1, \dots, q\}$  also denotes a  $p/q$ -section with  $v_0 = 0$  and  $v_q = p$ , these two sections must be replica of each other for  $\chi < \chi_q$ . Therefore, we have the following corollary.

**Corollary 3.** For  $\chi < \chi_q$ ,  $u_n + u_{q-n} = p$  holds for  $0 \leq n \leq q$  in a  $p/q$ -section with  $u_0 = 0$  and  $u_q = p$ .

### III. Sections and recurrent configurations

Consider a  $p/q$ -section with  $u_0 = 0$  and  $u_q = p$ . From Eq. (2.13), with  $l_k$  replaced by  $\gamma M_k$  for  $1 \leq k \leq q-1$  since none of them are pinned, one has

$$s_0 = p \csc q\chi - \gamma \csc q\chi \sum_{k=1}^{q-1} M_k \sin(q-k)\chi, \quad (3.1)$$

which leads to

$$\begin{aligned}
 u_n &= \frac{p}{2} \nu_q \cos \left( n - \frac{q}{2} \right) \chi + \frac{p}{2} \csc \frac{q\chi}{2} \sin \left( n - \frac{q}{2} \right) \chi + \nu_q \sum_{k=1}^{q-1} M_k \cos \left( |n-k| - \frac{q}{2} \right) \chi \quad (3.2) \\
 &= \nu_q \sum_{k=0}^{q-1} \left( M_{n+k} - M_k + \frac{1}{2} \delta_k^q - \frac{1}{2} \delta_{n+k}^q \right) \cos \left( k - \frac{q}{2} \right) \chi, \quad (3.3)
 \end{aligned}$$

where  $\nu_q \equiv \tan(\chi/2) \csc(q\chi/2)$  and  $\delta_k^q$  is the Kronecker delta function with module  $q$ ; i.e.,  $\delta_k^q$  equals 1, if  $k \equiv 0 \pmod{q}$  or 0, otherwise. Here a consequence of corollary 3,  $M_k + M_{q-k} = p$  for  $0 < k < q$ , is employed. One should note that Eq. (3.2) is valid for  $0 \leq n \leq q$ ; however, Eq. (3.3) is valid for any integer  $n$ . Namely, Eq. (3.3) describes a configuration with repetitious  $p/q$ -sections.

Consider the configuration described by Eq. (3.3). At  $\chi = 0$  one has  $u_n = np/q$  and  $M_k = \text{Int}[kp/q] + 1/2$ . As  $\chi$  increases,  $u_{nq}$  is fixed to  $np$  and all other  $u_k$ 's are continuous functions of  $\chi$  if all the values of  $M_k$  remain the same for each  $k$ . From the definition of  $M_k$ , one knows that the values of  $M_k$  can change only when  $u_k$  varies across an integer value. When  $u_k$  touches an integer value for  $k \not\equiv 0 \pmod{q}$ , a  $p/q$ -section will be divided into two different sections since  $p/q$  is irreducible. Form Corollary 2, this cannot happen for  $\chi < \chi_q$ . Therefore, we have the following corollary.

**Corollary 4** For a configuration composed of repetitious  $p/q$ -sections with  $u_0 = 0$ , one has  $\text{Int}[u_n] = \text{Int}[np/q]$  for  $\chi < \chi_q$ .

Actually, Eq. (3.2) can be used to describe a  $p/q$ -section up to  $\chi = \bar{\chi}_q \equiv \pi / \max(q_1^0, q_2^0)$ . However, for  $\chi_q < \chi \leq \bar{\chi}_q$ , it is a unstable resonance state according to Theorem 1.

Now let us consider the recurrent [14] configuration without atoms pinned at the cusps. Though these kinds of configurations cannot be of minimum energy, they, as we shall see, play the role of the reference configurations in deriving the system energy.

For a recurrent configuration with winding number  $p/q$  and none of the atoms being pinned, let us assign  $v_0$  to the atom which is closest to the nearest integer at its lefthand side and that integer point is set to  $u = 0$ . Assigning the position of the  $n$ -th atom, counting from  $v_0$ , as  $v_n$ , one has  $v_q = v_0 + p$  and a formal solution of this configuration is given by

$$\begin{aligned}
 v_0 &= c_0, \\
 v_1 &= c_0 \cos \chi + s_0 \sin \chi, \\
 v_2 &= c_0 \cos 2\chi + s_0 \sin 2\chi + \gamma N_1 \sin \chi, \\
 v_3 &= c_0 \cos 3\chi + s_0 \sin 3\chi + \gamma N_1 \sin 2\chi + \gamma N_2 \sin \chi, \\
 &\vdots \\
 v_q &= c_0 \cos q\chi + s_0 \sin q\chi + \gamma \sum_{k=1}^{q-1} N_k \sin(q-k)\chi
 \end{aligned}$$

with some suitable parameters,  $c_0$  and  $s_0$ , and  $N_k \equiv \text{Int}[v_k] + 1/2$ . Similar to the above case, one can use relations,  $v_q = v_u + p$  and  $v_{q+1} = v_1 + p$  to derive that

$$\begin{aligned} v_n &= \frac{p}{2} \nu_q \cos\left(n - \frac{q}{2}\right) \chi + \frac{p}{2} \csc \frac{q\chi}{2} \sin\left(n - \frac{q}{2}\right) \chi + \nu_q \sum_{k=0}^{q-1} N_k \cos\left(|n - k| - \frac{q}{2}\right) \chi \\ &= \nu_q \sum_{k=0}^{q-1} \left(N_{n+k} - N_k + \frac{1}{2} \delta_k\right) \cos\left(k - \frac{q}{2}\right) \chi, \end{aligned} \quad (3.4)$$

where  $\delta_k$  is the Kronecker delta function. One should note that Eq. (3.4) is valid for  $0 \leq n \leq q$  and Eq. (3.5) is valid for any integer  $n$ . At  $\chi = 0$ , one can assign  $\text{Int}[kp/q + 1/(2q)] + 1/2$  to  $N_k$ , which is valid until one of the atoms touches the cusps as  $\chi$  increases. This occurs at  $\chi = \chi_q$  where  $v_u = 0$  and  $v_{q_2} = p_2^0$ .

#### IV. Hull function and system energy

To calculate the system energy, it is convenient to introduce the hull function. Consider the reference recurrent configuration given by  $\{v_n\}$ . With winding number  $p/q$ , there are  $q$  allowable positions for atoms in each period of the potential and, therefore, the full function,  $f_\omega(x)$ , is composed of plateaux with widths  $1/q$ . We would like to fix the phase variable  $\alpha$  so that  $f_\omega(x) = v_0$  for  $0 \leq x < 1/q$ . To satisfy Eq. (1.4), one has

$$f_\omega(x) = \nu_q \sum_{k=0}^{q-1} \left(\text{Int}[x + k\omega] - \text{Int}[k\omega] + \frac{1}{2} \delta_k\right) \cos\left(k - \frac{q}{2}\right) \chi. \quad (4.1)$$

The average energy per atom,  $\Psi(\omega)$ , of this recurrent configuration is given by

$$\begin{aligned} \Psi(\omega) &= \int_0^1 dx \left\{ -\frac{\lambda}{2} \left[ f_\omega(x) - \frac{1}{2} \right]^2 + \frac{1}{4} [f_\omega(x + \omega) - f_\omega(x)]^2 + \frac{1}{4} [f_\omega(x) - f_\omega(x - \omega)]^2 \right\} \\ &= \frac{\omega^2}{2} + \frac{\lambda}{4} \int_0^1 dx (1 - 2x) f_\omega(x) \\ &= \frac{\omega^2}{2} - \frac{\lambda}{4} \nu_q \sum_{k=0}^{q-1} \left\{ \frac{1}{4} - \left( k\omega - \text{Int}[k\omega] - \frac{1}{2} \right)^2 \right\} \cos\left(k - \frac{q}{2}\right) \chi, \end{aligned} \quad (4.2)$$

where the fact that  $f_\omega(x) - x$  is periodic in  $x$  and the relation,

$$\int_0^1 dx (1 - 2x) (\text{Int}[x + \alpha] - \text{Int}[\alpha]) = (\alpha - \text{Int}[\alpha])^2 - (\alpha - \text{Int}[\alpha]), \quad (4.3)$$

are employed. It is interesting to note that if we regard  $\kappa q$  atoms in  $\kappa p$  wells as a large molecule, the energy per atom is also expressible as

$$\Psi(\omega) = \frac{\omega^2}{2} - \frac{\lambda}{4} \nu_{\kappa q} \sum_{k=0}^{\kappa q - 1} \left\{ \frac{1}{4} - \left( k\omega - \text{Int}[k\omega] - \frac{1}{2} \right)^2 \right\} \cos\left(k - \frac{\kappa q}{2}\right) \chi. \quad (4.4)$$

In addition, Eqs. (3.5) and (3.3) are also expressible as

$$v_n = \nu_{\kappa q} \sum_{k=0}^{\kappa q-1} \left( N_{n+k} - N_k + \frac{1}{2} \delta_k^q \right) \cos \left( k - \frac{\kappa q}{2} \right) \chi \quad (4.5)$$

and

$$u_n = \nu_{\kappa q} \sum_{k=0}^{\kappa q-1} \left( M_{n+k} - M_k + \frac{1}{2} \delta_k^q - \frac{1}{2} \delta_{n+k}^q \right) \cos \left( k - \frac{\kappa q}{2} \right) \chi. \quad (4.6)$$

Similarly, a configuration with repetitious  $p/q$ -sections can be described by the hull function,

$$f_\omega(x) = \nu_q \sum_{k=0}^{q-1} \left( \frac{1}{2} \text{Int} \left[ x + k\omega + \frac{1}{2q} \right] + \frac{1}{2} \text{Int} \left[ x + k\omega - \frac{1}{2q} \right] - \text{Int}[k\omega] + \frac{1}{2} \delta_k \right) \times \cos \left( k - \frac{q}{2} \right) \chi \quad (4.7)$$

where the phase variable  $\alpha$  is chosen to make  $f_\omega(x) = u_0$  for  $-1/(2q) \leq x < 1/(2q)$ . The average energy per atom,  $\Psi_e(\omega)$  of this section is given by

$$\Psi_e(\omega) = \Psi(\omega) - \frac{\lambda}{8} \nu_q \cos \frac{q}{2} \chi. \quad (4.8)$$

For any  $\lambda > 0$ , there must be some positive integer  $q_c$  such that  $\chi_{q_c+1} < \chi \leq \chi_{q_c}$ . Only those  $w$ -sections with  $\omega$  in the  $q_c$ -th row of the Farey fractions need be taken into account in searching for the minimum energy configurations. To keep the winding number fixed, we only need to compare the energy sectionally; namely, to derive the energy difference of  $\kappa$   $p/q$ -sections with a  $p_1/q_1$ - and a  $p_2/q_2$ -section. The energy differences in the general case can be obtained with summation over successive energy differences of this kind.

Consider any segment of  $\kappa q + 1$  atoms,  $\{u'_0, u'_1, \dots, u'_{\kappa q}\}$ , with  $u'_{\kappa q} = u'_0 + \kappa p$ . One can define  $M'_n \equiv \text{Int}[u'_n] + 1/2$  and  $\lambda \tilde{M}'_n \equiv u'_{n+1} + u'_{n-1} - (2 - \lambda)u'_n$ . If  $\lambda \tilde{M}'_n - \lambda M'_n \neq 0$ , the difference is either the pinning force to keep  $u'_n$  pinned at a cusp or the external force, needed to keep  $u'_n$  staying at a non-stationary position. The energy of such a segment is given by

$$\begin{aligned} \kappa q \Psi'(\omega) &= \sum_{k=0}^{\kappa q-1} \left[ \frac{1}{2} (u'_{k+1} - u'_k)^2 - \frac{\lambda}{2} (u'_k - M'_k)^2 \right] \\ &= \kappa q \Psi(\omega) + \frac{\lambda}{2} \sum_{k=0}^{\kappa q-1} \left[ (u'_k - v_k)(2M'_k - N_k - M'_k) \right. \\ &\quad \left. + (N_k - M'_k)(M'_k + N_k - 2u'_k) \right]. \end{aligned} \quad (4.9)$$

A segment composed of a  $p_2/q_2$ -section and a  $p_1/q_1$ -section can be described with

$$u'_n = \nu_{\kappa q} \sum_{k=0}^{\kappa q-1} \left( M'_{n+k} - M'_k - \frac{1}{2} \delta_k^q + \beta \delta_{k+n}^{\kappa q} - \beta \delta_{k+n-q_2}^{\kappa q} \right) \cos \left( k - \frac{\kappa q}{2} \right) \chi \quad (4.10)$$

for  $0 \leq n \leq \kappa q$ , where  $\beta \equiv \cos(\kappa q \chi / 2) \csc(q_1 \chi / 2) \csc(q_2 \chi / 2) / 4$  and  $M'_k = N_k$  for any  $k$ . Therefore, the last term on the righthand side of Eq. (4.9) vanishes and the energy can be derived easily. As compared with Eq. (4.8), one has

$$q_1 \Psi_e(\omega_1) + q_2 \Psi_e(\omega_2) - \kappa q \Psi_e(\omega) = \frac{\lambda}{8} \tan \frac{\chi}{2} \cot \frac{q\chi}{2} \tan \frac{q_1 \chi}{2} \tan \frac{q_2 \chi}{2}. \quad (4.11)$$

## V. Ground state configuration

One notes that the righthand side of Eq. (4.11) is always positive for  $\chi < \pi / \max(q, q_1, q_2)$ . This indicates that for  $0 < \chi < \chi_q$ , the ground state configuration with winding number  $w = p/q$  is given by the one composed of  $p/q$ -sections. Furthermore, the average energy per atom is a convex function of those fractions in the  $q_c$ -th row of Farey fractions.

At  $\chi = \chi_q$ ,  $q_c = q$ ,  $\kappa = 1$ ,  $\omega_1 = \omega_1^0$ ,  $\omega_2 = \omega_2^0$ , and the righthand side of Eq. (4.11) equals zero. Namely, a  $w$ -section can dissociate into one  $\omega_1^0$ - and one  $\omega_2^0$ -section without costing any energy. This process can be done through a zero frequency mode,  $\delta u_k = a \sin k \chi_q$  for  $0 \leq k \leq q$ . The amplitude  $a$  is restricted so that the in-between particles,  $\{u_1, u_2, \dots, u_{q-1}\}$ , can only barely touch the cusps and Eq. (1.2) still holds for them. The extreme case happens when either  $u_{q_1^0} = p_1^0$  or  $u_{q_2^0} = p_2^0$ . In either case, the  $w$ -section has dissociated into one  $\omega_1^0$ - and one  $\omega_2^0$ -section. For  $\chi > \chi_q$ , the  $w$ -section is unstable according to Theorem I and it dissociates into  $\omega_1^0$ - and  $\omega_2^0$ -sections completely. One should note that arbitrary spatial ordering of these  $\omega_1^0$ - and  $\omega_2^0$ -sections won't lead to any difference in energy; therefore, this ground state configuration is highly degenerate.

For a general winding number not in the  $q_c$ -th row of Farey fractions, the minimum energy configurations must be composed of different kinds of sections. Consider  $p_a/q_a < p_b/q_b$  to be non-successive fractions in the  $q_c$ -th row of Farey fractions. Assume there are both  $p_a/q_a$ - and  $p_b/q_b$ -sections in a stationary configuration. By interchanging them with other sections and moving them rigidly, they can be placed next to each other without changing the energy of this configuration. One can find an irreducible  $p/q$  such that  $\kappa' p = p_a + p_b$  and  $\kappa' q = q_a + q_b$  with some positive integer  $\kappa'$  and  $p_a/q_a < p/q < p_b/q_b$ . If  $p/q$  is in the  $q_c$ -th row of Farey fractions, then transforming the consecutive  $p_a/q_a$ - and  $p_b/q_b$ -sections into  $\kappa'$   $p/q$ -sections will lower the energy. If not, we can find a unique pair of successive fractions in the  $q_c$ -th row of Farey fractions,  $p_1/q_1 < p_2/q_2$ , such that  $p = \kappa_1 p_1 + \kappa_2 p_2$  and  $q = \kappa_1 q_1 + \kappa_2 q_2$  with some positive integers,  $\kappa_1$  and  $\kappa_2$ , and there must be either  $p_a/q_a < p_1/q_1$  or  $p_2/q_2 < p_b/q_b$ . From Eq. (4.11), transforming the consecutive  $p_a/q_a$ - and  $p_b/q_b$ -sections into  $\kappa' \kappa_1 p_1/q_1$ -sections and  $\kappa' \kappa_2 p_2/q_2$ -sections will lower the energy. Therefore, we have the following theorem.

**Theorem III** In the *FK model* determined by Eqs. (1.2), (2.1), and (2.3) with  $\chi_{q_{c+1}} < \chi \leq \chi_{q_c}$ , the minimum energy configuration can be composed of at most two kinds of sections with their corresponding fractions being successive in the  $q_c$ -th row of Farey fractions.

In summary, for given  $\chi$ , there exists a positive integer  $q_c$  such that  $\pi/(q_c+1) < \chi \leq \pi/q_c$ . The ground state configurations can only be composed of the  $w$ -sections with  $\omega$  in the  $q_c$ -th row of Farey fractions in the following way. For an arbitrary irrational winding number  $w$  or rational but not in the  $q_c$ -th row of Farey fractions, we can find a unique pair of consecutive fractions  $\omega_1$  and  $\omega_2$  in the  $q_c$ -th row of Farey fractions such that  $\omega_1 < w < \omega_2$ . The ground state configuration with this given  $w$  can be constructed with a fraction  $\mathbf{f}_1$  of particles associated with the  $w$ -sections and a fraction  $\mathbf{f}_2$  associated with  $\omega_2$ -sections such that

$$\mathbf{f}_1 + \mathbf{f}_2 = 1, \quad (5.1)$$

and

$$\mathbf{f}_1\omega_1 + \mathbf{f}_2\omega_2 = \omega. \quad (5.2)$$

More specifically, the ground state configuration is composed of  $\omega_1$ - and  $w$ -sections with their abundance in the ratio  $\mathbf{f}_1q_2 : \mathbf{f}_2q_1$ . The average energy per atom in this configuration is given by

$$\Psi_e(\omega) = \frac{\omega_2 - \omega}{\omega_2 - \omega_1} \Psi_e(\omega_1) + \frac{\omega - \omega_1}{\omega_2 - \omega_1} \Psi_e(\omega_2). \quad (5.3)$$

It should be noted that for  $w$  in the  $q_c$ -th row of the Farey fractions, the energy is given by Eq. (4.8) and for all the other winding numbers, the energy is given by Eq. (5.3). Eq. (4.11) thus indicates that  $\Psi_e(\omega)$  is a convex function of  $w$ . Furthermore, these  $\omega_1$ - and  $w$ -sections can be arranged in an arbitrary spatial order. Therefore, the ground state configuration with winding number  $w$  is highly degenerate.

Here we would like to elaborate on the ground state configurations and the minimum energy configurations. For a given  $\lambda$  and an accompanying  $q_c$ , if the winding number is fixed at a value not in the  $q_c$ -th row of Farey fractions, then the ground state configurations are highly degenerate and there are no other distinguishable minimum energy configurations. If the winding number is fixed at a value,  $w$ , in the  $q_c$ -th row of Farey fractions, the ground state configuration is composed solely of  $w$ -sections. However, according to the definition in [6], a minimum energy configuration allows of a finite number of either  $\omega_1$ -sections (solitons) or  $w$ -sections (anti-solitons), but not a mix of them, being created, in consistent with Theorem III.

It is interesting to note that it is not even necessary for a minimum energy configuration of this model to have a well-defined winding number. For example, assuming  $\omega_1$  and  $\omega_2$  to be any consecutive fractions in the  $q_c$ -th row of Farey fractions, one can, starting from  $u = 0$  to both sides, put  $2^0$   $\omega_1$ -section, then adding  $2^1$   $w$ -sections, then  $2^2$   $\omega_1$ -sections,  $2^3$   $\omega_2$ -sections,  $\dots$ , and so forth. The winding number defined in Eq. (1.3) doesn't have a well-defined value for this configuration. Therefore, some of Aubry's results [6] for a minimum energy configuration don't apply in this case.

Up to now, we have been discussing the minimum energy configuration for given  $w$  as  $\chi$  is varied. Introducing the tensile force term  $-\sigma\omega$  into Eq. (4.2), we obtain the enthalpy of this system. By minimizing this enthalpy with respect to  $w$ , we obtain the function showing

the periodicity,  $\omega$ , versus the the tensile force,  $\sigma$ . From the above discussion, we know this function is composed of plateaux corresponding to winding numbers in the  $q_c$ -th row of Farey fractions with  $q_c$  determined by  $\lambda$ . The width of  $\sigma$  corresponding to all the other winding numbers has zero measure. Therefore, the structure of this function is a harmless staircase.

## VI. Conclusions

We have presented an exactly solved model which exhibits the harmless staircase. All the mathematical details needed to completely characterize the minimum energy configurations and the ground state configurations are rigorously established. Our method should be applicable to quite a general case of FK models with potentials almost everywhere concave and have cusps at the bottom.

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