

# Comment on “Out-of-equilibrium Frenkel-Kontorova model” by A. Imparato 2021 J. Stat. Mech. 013214

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**Abstract** We explain the ‘phases’ of a Frenkel-Kontorova chain of atoms in a different way to the commented article. We reject the decision of states of the chain into commensurate and incommensurate states introduced by S. Aubry.

**Keywords** Frenkel-Kontorova model · Phase · Average particle-particle distance · Tilted potential · JSTAT

## 1 Introduction

This paper is devoted to the aim of understanding what happens inside the finite Frenkel-Kontorova (FK) chain, if the two ratios  $a/b$  and  $V_o/k$  change. The corresponding model of a linear FK chain  $\mathbf{x} = (x_1, \dots, x_N)$  with atoms of equal mass at points  $x_i$  is [1]

$$U(\mathbf{x}) = -V_o \sum_{i=1}^N \cos\left(\frac{2\pi}{b} x_i\right) + \frac{k}{2} \sum_{i=1}^{N-1} (x_{i+1} - x_i - a)^2. \quad (1)$$

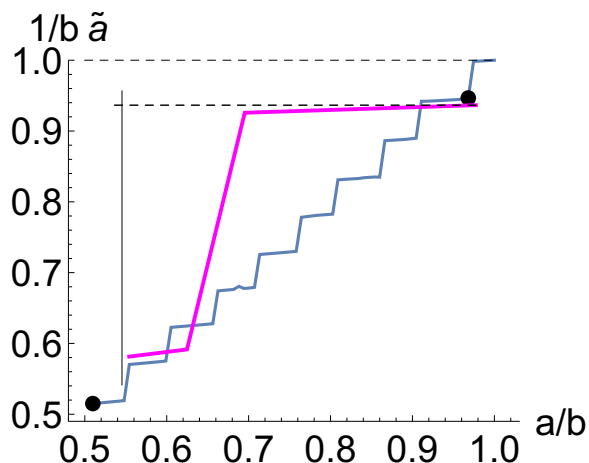
$V_o$  describes the strongness of the substrate, but  $k$  the elastic spring forces between neighboured atoms. Parameter  $b$  is the periodicity of the substrate. It is used throughout with  $2\pi$ . The boundary conditions for  $x_1$  and  $x_N$  are free. Parameter  $a$  is the distance of two atoms if the parameter  $V_o$  would be zero. However, in

the chain with the substrate potential,  $V_o \neq 0$ , the average distance,  $\tilde{a}$ , usually changes

$$\tilde{a} = \frac{x_N - x_1}{N - 1}. \quad (2)$$

## 2 Comment

Our first remark concerns the ansatz of Eq.(3) in Ref. [1], our Eq.(2). There are  $(N-1)$  distances between the particles  $x_N$  and  $x_1$ . The false use of  $N$  makes the lowering of the line at 1 by  $1/20$  in Fig.1 in [1], and a row of crude factors  $(N-1)/N$  there. We give a new point of view on the problem of taking the limit  $N \rightarrow \infty$  below.



**Fig. 1** Plot of a staircase of the average particle-particle distances for  $N=20$ ,  $k=5$ ,  $V_o=5$  somewhat similar to Fig.1 in [1] however with more steps. In contrast to [1] we find quasi regular steps. We avoid noise for the pure chain without temperature, to understand the structures of the minima. The special chains at the bullets are depicted in the next Figures. The magenta overlay of the inner picture magnifies the first step showing that its slope is not zero.

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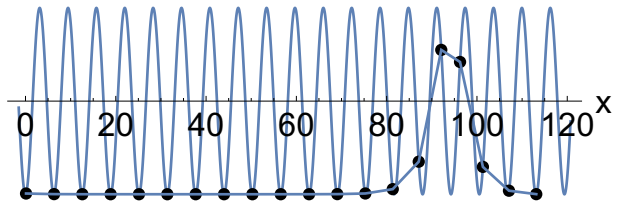
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Our main remark concerns the discussion of commensurate or incommensurate states of the chain. We start with the chain at the potential energy (1) without noise thus the possibility to smear out some structures by statistics. We determine the pure minimizer of the chain in the combined two potentials (1), by the substrate and by the elastic forces. We have recalculated a part of the curve like in Fig.1 of [1]. The result is shown in our Fig. 1. The calculations are done with a step length of 0.04 thus 78 calculations are executed for  $a_s = b - s * 0.04$  for the stepnumbers  $s = 0, \dots, 78$  in the  $b/2$  interval (with  $b = 2\pi$ ). The initial chain of every optimization is one with  $x_1$  at zero and  $x_i = i a$ . The minima of the FK-chain with  $N = 20$  atoms disclose 10 steps in the region  $0.5 \leq a/b \leq 1$ , quite more than the coarse statistics of ref. [1] can do.

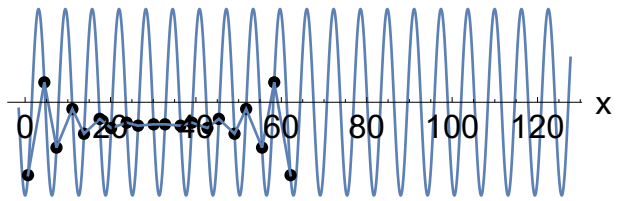
The step at  $\tilde{a}/b \approx 1$  is reproduced, only rational numbers are used for the full step. The step near the dashed line 1 is not constant; it decreases very slowly to the left hand side, compare the inset in Fig.1. Thus we conclude that the statement that there is a “zero slope of length  $\Delta$ ” [2] is not correct. The decrease comes from a small ascent of the  $\approx N/2$  left atoms to the right walls of their corresponding substrate potential wells, and of the  $\approx N/2$  right atoms to the left walls of their corresponding substrate potential wells, what shortens  $\tilde{a}$ . The jump down to the upper bullet in Fig. 1 is explainable by the structure of the chain in Fig. 2. Note that this fact does not have relations with commensurate, or incommensurate numbers. The key is that the outer atom,  $x_N$ , jumps over the outer peak of the site-up potential at the end of the upper step of the staircase. This pattern repeats for smaller values of  $a/b$  again and again at every step. So the jumps emerge in Fig.1.

From Cantor’s proof that the real numbers are uncountable but the rational numbers are countable, it follows that almost all real numbers are irrational. But the rational numbers are as dense as the irrational ones. (See any textbook for a first course in Analysis.) There is no gap in both kinds of numbers which indicates the steps in Fig.1 of [1]. We conclude that to relate the transition of different phases of the FK-chain with the transition from a rational to an irrational ratio of  $\tilde{a}/b$  is mathematically and also physically not correct.

The adsorption [2] of the chain by the substrate acts in the kind that for every ratio  $a/b$  a rational  $\tilde{a}$  emerges (to every given exactness of the solution) for a minimum structure, if  $N$  is finite. The latter was our assumption because in physics only finite chains exist. The claimed limit  $N \rightarrow \infty$  in [1,2] is a mathematical abstraction. Thus one can assume that to every constellation of the parameters  $a/b$ ,  $V_o/k$ , and  $N$ , exists at least one mini-



**Fig. 2** Minimum structure at the upper bullet of Fig. 1, at  $a/b = 0.968$ , for  $N=20$ ,  $k=5$ ,  $V_o=5$ , and no noise. After a great jump downhill to the left hand side, the chain is shortened by one well. Note that the atoms in the figure are artificially lifted on the substrate potential to guide the eye. The real chain is on a straight line. Only the distances can change. The spring potential is not shown in the scheme.



**Fig. 3** Minimum structure at the left lower bullet of Fig. 1 for  $N=20$ ,  $k=5$ ,  $V_o=5$ , and no noise. The chain is shortened to a lower number of  $N/2 + 1$  wells of the site-up potential. Note the fully symmetric structure of the chain.

mizer, a structure of the FK chain in a minimum of the combined potential (1). We explicitly define different ‘phases’ of the chain:

#### DEFINITION

If an equilibrium structure of the FK-chain occupies  $L$  wells of the substrate then it belongs to phase  $L$ . There is a certain set of parameters for different ratios of  $a/b$ ,  $V_o/k$ , and  $N$ , which lead to the same phase. A single phase transition is correspondingly a change of an equilibrium structure of the FK-chain to  $L + 1$  or  $L - 1$  wells.

(A strong definition what is a ‘phase’ of an FK model is missing in [1,2].) For a phase transition the whole chain contracts, or expands, so that one or more atoms of the chain climb over their current peaks of the substrate potential. As a result, the chain uses less, or more wells. It is connected by a jump in the average  $\tilde{a}$ , compare Figs. 1-3. The question circles around the count of integers, whole numbers which one counts with the fingers. The putative sophistication of treatments with ‘incommensurable’ FK states has obscured the simplicity of this central point.

Besides the ratio of  $a/b$  the balance of  $k$  and  $V_o$  also plays an important role. This is correctly described in [1] by the comparison of the ‘length’ of the first phase, see Fig.1a of [1], for  $V_o = 1, 5$ , or  $10$  under an equal  $k$ -parameter.

Often the jumps in Fig. 1 are named 'discontinuations' [1,2] of the chain. We emphasize that the order of the chain will rather be conserved. Only some distances change stronger, as well as  $\tilde{a}$ . But note that the balance of the substrate potential as well as the elastic forces of the FK model acts over all atoms of the chain.

The chain of Fig. 2 contains an antikink, a compressed structure, which can wander through the chain and which can perform an internal movement [3]. Its location is somewhat accidental. The contraction of a smaller part of the chain in the antikink is not an incommensurate ratio in the sense of the definition [2] by an irrational number. Note that there exist low energy saddle points [3] in between over which the internal movement of parts of the chain goes on as a solitone. Every new lower step of the staircase of Fig. 1 is formed by an additional antikink resulting in a new phase.

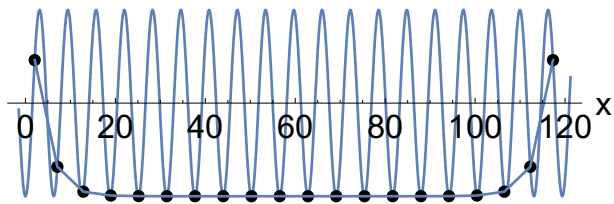
The chain of Fig. 3 is a regular structure, no kind of incommensurability emerges at  $a/b \approx 1/2$  like it is claimed in [1]. The two outer atoms have a single well, but all other atoms are distributed by two per well. Though quite regular, the two atoms per well are not at the bottom of the substrate [1,2] because they are repulsed vice versa by their elastic forces. Note that no atom sits at the bottom of the substrate. This has important consequences, compare the end of section 3.

In [1] is not discussed that different global minimizers with different  $\tilde{a}$  may exist to a given  $N$ . Compare the case  $N=8$ ,  $a/b=1/2$  in Fig. 6 of ref. [3].

For the first step of another staircase longer than in Fig. 1 a set of minima exists where, in contrast to Fig. 2 the outer two atoms,  $x_1$  and  $x_N$ , symmetrically climb up on their outer walls of the substrate. The minimum of a current result for parameter  $a_s = 2\pi - 0.04s$  is taken for the initial chain of the next optimization. These structures exist up to  $a/b \approx 0.68$  and  $\tilde{a} < 1$  but near to 1. Thus, the first step of a staircase can be quite longer than in Fig. 1 as it may be the case in Fig. 1a of [1]. We show a structure of this kind in Fig. 4. If the atoms  $x_1$  and  $x_N$  climb uphill in their corresponding wells then continuously the  $\tilde{a}$  decreases but  $L$  is not changed. The step of a staircase for this  $L$  also has a nonzero slope.

The examples demonstrate that one and the same set of parameters,  $a/b$  and  $V_o/k$ , can belong to different phases, thus can have a different  $\tilde{a}$ .

We still treat the case  $N \rightarrow \infty$ . The finite case only is treated in Ref. [1], from  $N = 20$  to  $N = 1000$ , though  $\tilde{a}$  is defined by the limit. Possibly the trend of the  $\tilde{a}$ -values is not monotone. In the case  $a/b=2/3$  in paper [3], Fig. 2, there the  $\tilde{a}$  jumps for integers of  $N/3$  for increasing  $N$ . In Fig. 7 in [3],  $\tilde{a}$  jumps for  $a/b=1/2$  from



**Fig. 4** Minimum structure at the upper step of a staircase for  $N=20$ ,  $k=5$ ,  $V_o=5$ , and no noise, compare Fig. 2. The chain is still not shortened to a lower number of wells of the site-up potential, see text.

$N=10$  to 11 to 12. However, this flattens out for large  $N$ .

We find that the larger  $N$  is, the 'earlier' a small change in parameter  $a$  leads to a change of the number of occupied wells. That is because the unperturbed chain ends at  $x_N = (N - 1)a$ . If the shortening overcomes to an

$$a \approx b - \frac{Mb}{N-1} \quad (3)$$

with a certain small integer  $M > 0$  depending on  $V_o$  and  $k$ , then the count of the wells for a global minimum of the chain may jump to a lower number. In our case,  $N = 20$ , and  $V_o = k$ ,  $M = 1$  is enough to overcome the step length of  $a/b \approx 0.025$  of the first upper step. However, for larger and larger  $N$ , the limit treatment, formula (3) leads to the decrease of the step length to zero. The staircase of Fig. 1 degrades to a straight line. Independent of the (finite) parameters  $V_o$  and  $k$ , any kind of "devils staircase" [1,2] disappears in the limit but the relation of  $\tilde{a}$  to  $a$  forms a straight line. There is  $\tilde{a} = a$  throughout.

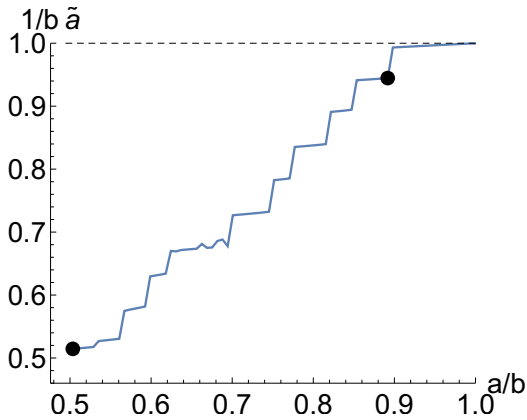
### 3 The use of Temperature

Eq.(4) of ref. [1] introduces the temperature. In the spirit of ref. [4] we can understand the periodic noise as a tilting to the site-up potential (1) by a corresponding constant force vector,  $\mathbf{F}$ . Thus we treat the linearly tilted potential

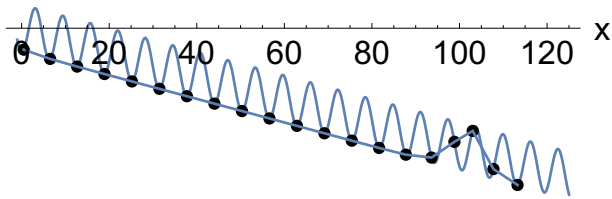
$$U(\mathbf{x}) - \mathbf{F} \mathbf{x}^T \quad (4)$$

with  $\mathbf{F} = F(1, \dots, 1)$ . It is of interest to find first the true minima of the chain under a tilting too. This is demonstrated in Figs. 5-7 with  $F = 0.25$ . (We compared the  $T$ -values of [1] with the factor of the white noise being usually absolutely lower than 0.2. It gives the coarse approximation of 0.25.) We search again for minima of the chain under such a mild tilting. We use the optimization order in the Mathematica program. Resulting structures of the FK chain are now not symmetric, compare Figs. 6 and 7. Over  $1/2 \leq a/b \leq 1$  we

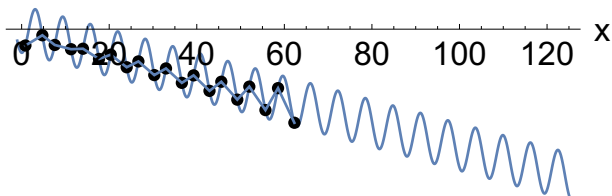
get stable minimum structures. The chain is still pinned and no sliding of the full chain happens.



**Fig. 5** Plot of the staircase of average particle-particle distances for  $N=20$ ,  $k=5$ ,  $V_o=5$ , and a tilting of  $F = 0.25$ . The structure of the chain at the two bullets is shown in Figs. 6 and 7.



**Fig. 6** Minimum structure at the upper bullet of Fig. 5, for  $N=20$ ,  $k=5$ ,  $V_o=5$ , and tilting  $F = 0.25$ . The shortening of the  $a$  parameter causes a jump analogously to Fig. 2 by forming of a skew antikink. The chain is shortened to  $N - 1$  wells of the site-up potential.



**Fig. 7** Minimum structure at the lower bullet of Fig. 5, for  $N=20$ ,  $k=5$ ,  $V_o=5$ , and tilting 0.25. Because  $\bar{a}/b \approx 1/2$ , we again find a quasi regular minimum with two atoms per well of the site-up potential, without the two outer atoms which individually occupy a well. Note that it is not a kind of incommensurability.

A stronger tilting results in many upper steps of the  $\bar{a}/b$  curve, like in Figs. 1 and 5. The steps describe stable, pinned minima of the chain. However, anywhere the leftmost atom,  $x_1$ , climbs to the right hand side

over the top of its substrate peak. But then a next minimum does not appear. The next jump to a shorter structure leads to a total depinning of the chain. The tilted potential becomes an overhang [2]. Then no minimum structure is obtained. The chain slides down the tilted substrate with a velocity as it is reported in [1]. It is to assume that the free sliding chain assumes its  $a$ -distances. This is to observe in Fig. 1 of [1] in the step-free parts of the curves. The influence of the substrate disappears. The chain is more or less free moving. May be it can vibrate under the sliding.

The remaining steps in Fig. 1 of [1] describe the pinned region of the parameter space. But a discussion of pinned structures is missing in [1], as well as a discussion of the transition to depinning. The depinned chain slides over possible saddle points and intermediate minima of the potential which exist for tiltings [3].

The example of Fig. 7 is again a quite regular structure of the chain, no kind of incommensurability emerges at  $a/b \approx 1/2$  as it is claimed in [1]. Though quite regular, two atoms per well are not at the bottom of the substrate [1] because they are repulsed vice versa by their elastic forces. This has important consequences, compare the end of this section. The cases of pinned structures like in Figs. 6 and 7 are not discussed in [1] though in some of the Figures in [1] emerges a zero velocity. It points to pinned structures.

The minima of the linearly tilted potential in eq.(4) are not the full picture of the Kramer's equation (5) in [1]. If one includes the vibration term, one has a more complicated picture, like in [1]. Nevertheless, a comparison with our pinned structures may be of interest. In the case of a depinning, especially the question emerges why the velocity,  $\bar{v}$ , of the chain becomes so large near the parameter combination  $a/b \approx 1/2$ ? Of course,  $1/2$  is not incommensurable to 1. So, the reasoning in [1], Fig. 1a, that there one has a maximal IC-phase, does not fit the problem. Most results in [1] are given for  $\Phi_T = \pi/2$ . For  $a/b \approx 1$ , all atoms are sitting in the minima of the site-up potential. Their 'hot spots' of the temperature,  $T(\mathbf{x})$  in eq.(4) of [1], at  $(x_i + \pi/2)$  are 'far away' by  $\pi/2$  from the tops of the barriers of the site-up potential. However, for  $a/b \approx 1/2$ , nearly a half of the atoms are sitting so at the slope that their 'hot spots' are near the tops of the barriers, compare our Figs. 3 and 7. We guess that these special atoms are moved by the Büttiker-Landauer process [4], and so the full FK chain is moved.

## 4 Conclusion

This comment discusses the widespread theory of so-called commensurate (C) versus incommensurate (IC) phases of the FK model [1,2]. We have seen that the so-called C-phases, the steps in Fig. 1, are not specially ordered phases in the sense that all atoms are locked-in to the minima of the substrate. In the putative IC-phases we also find no broken regular arrangement of the atoms of the chain. What makes steps in the average distance  $\tilde{a}$  of the chain is the possibility that the chain contracts or stretches over different periods  $L$  of the substrate. Of course we have to assume free boundaries of the chain.

In a 2D or 3D crystal lattice a long-range periodic order with an irrational ratio of the periodicities can exist [2]. Its description as an IC crystal is alright. However, the  $\tilde{a}$  in the FK model is not the description of a fixed lattice. It is rather the result of the balance of the four different parameters,  $a$ ,  $b$ ,  $V_o$ ,  $k$ , and it is only an average value. The term IC means 'out of proportion'. However, in the FK chain we have to sort  $N$  atoms into  $L$  wells of the substrate, both  $N$  and  $L$  are integers. Two integers always form a proportion, thus the coined term 'IC' is a wrong term. One should use the already introduced terms kink and antikink.

The point of  $a/b$  where the 'phase' transition occurs, thus the chain contracts to a smaller number of wells of the site-up potential, has nothing to do with rational or irrational numbers. It is the balance between the two forces of the FK model, and of their periodicities.

The steps in Fig. 1 are not flat, in contrast to a statement of ref.[2]. Water could drain off from the staircase. There is not a single value of  $\tilde{a}/b$  involved, but many different, slowly decreasing ratios, down to the jump point. This jump point is, in all of our calculations, of course a rational number because we use a computer working with rational numbers.

Final note: One of the origins of the incorrect 'C-IC sight' may be the articles of S. Aubry. We have given an analysis of a main part of his incorrect theory in Ref. [5].

Last remark: Refs. 1 and 2 in [1] cite the authors in an incorrect order, see references [6,7].

## Acknowledgement

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## Authors' contributions

All authors contributed equally to the paper.

## References

- [1] Imparato A 2021 *J. Stat. Mech.* 013214
- [2] Chaikin P M and Lubensky T C 1995 *Principles of Condensed Matter Physics.* (Cambridge: Cambridge University Press)
- [3] Quapp W, Bofill J M 2019 *Eur. Phys. J B* 92, 193
- [4] Büttiker M 1987 *Z. Phys. B* 68, 161-167
- [5] Quapp W, Bofill J M 2019 *Mol. Phys.* 117, 1541-1558
- [6] Kontorova T A, Frenkel Ya I 1938 *Zh. Eksp. Teor. Fis.* 8, 89-95 (in Russian).
- [7] Kontorova T A, Frenkel Ya I 1938 *Zh. Eksp. Teor. Fis.* 8, 1340-1348 (in Russian).