electronics

MDPI

Article

An Analysis of Some Properties and the Use of the Twist Map for the Finite Frenkel–Kontorova Model

Wolfgang Quapp [1,*] and Josep Maria Bofill [2,3]

[1] Mathematisches Institut, Universität Leipzig, D-04009 Leipzig, Germany
[2] Departament de Química Orgánica, Universitat de Barcelona, 08028 Barcelona, Spain
[3] Institut de Química Teórica i Computacional, Universitat de Barcelona, (IQTCUB), Martí i Franqués, 1, 08028 Barcelona, Spain
* Correspondence: quapp@math.uni-leipzig.de or quapp@uni-leipzig.de

Abstract: We discuss the twist map, with a special interest in its use for the finite Frenkel–Kontorova model. We explain the meaning of the tensile force in some proposed models. We demonstrate that the application of the twist map for the finite FK model is not correct, because the procedure ignores the necessary boundary conditions.

Keywords: Frenkel–Kontorova model; average distance; finite chain; tensile force; twist map

Citation: Quapp, W.; Bofill, J.M. An Analysis of Some Properties and the Use of the Twist Map for the Finite Frenkel–Kontorova Model. *Electronics* **2022**, *11*, 3295. https://doi.org/10.3390/electronics11203295

Academic Editor: Lucas Lamata

Received: 20 September 2022
Accepted: 10 October 2022
Published: 13 October 2022

1. Introduction

The Frenkel–Kontorova model (FK) was proposed in 1938 to discuss dislocations in a chain of particles [1]. In the last century, many aspects of solid-state physics have been discussed using the FK model as an example. One divides a set of particles into a one-dimensional subsystem of interacting elements and a remainder as a substrate. The latter acts on the extracted subsystem by a potential. Of special interest may be electronic applications [2–7] for Wigner electrons or Josephson junctions. Further models are charge-density wave conductors [8–10], charge transport in solids and on crystal surfaces [11], magnetic or ferro- and antiferromagnetic domain walls [12], magnetic superlattices [13], superconductivity [14,15], and vortex matter [16–18], to name a few.

The FK model for a chain of N particles (called atoms) at positions u_i on an axis has the energy [1,19]

$$U(\mathbf{u}) = \sum_{i=1}^{N} \lambda\, V(u_i) + \sum_{i=1}^{N-1} \frac{k}{2}(u_{i+1} - u_i - a_o)^2\,. \tag{1}$$

The substrate potential function is the usual one

$$V(u_i) = 1 - \cos\Big(\frac{2\,\pi}{a_s} u_i\Big)\,.$$

The parameter a_s is the period of this potential, and λ is its amplitude. The second term is the spring term for the nearest neighbor forces between the atoms. Parameter k is its amount. The equilibrium distance, a_o, of the chain would hold without the potential V, thus for $\lambda = 0$. Usually, the two periods a_o and a_s are different [20].

Sometimes the equilibrium distance, a_o, of the chain is missing [21–23]. At first, one has to assume that $a_o = 0$ is used. One treats the FK model as a different one with the pure harmonic potential of the spring forces between the nearest neighbors but often with an additional linear tensile force of amount μ

$$\sum_{i=1}^{N-1} \Big[\frac{k}{2}(u_{i+1} - u_i)^2 - \mu\,(u_{i+1} - u_i)\Big]\,. \tag{2}$$

Note that the alternating tensile force of form (2) reduces to two summands

$$-\mu\,(u_N - u_1)\,.$$

If $\mu = 0$, then putting all $u_i = 0$ (or putting all $u_i = n\,a_s$ with an integer n) gives zero energy [24–26]. This is the global minimum, but it is a trivial one. If one starts with any finite chain with no zero distances between the atoms, and if one uses the values of the parameters of ref. [21] for $\lambda \leq k$, and $\mu = 0$, then a minimization would return this trivial result.

In Appendix A, we remark that for $\lambda \gg k$, further stationary states can exist for $a_o = 0$ and for $\mu = 0$. However, these states are not global minima.

The paper mainly discusses the application of the twist map on a finite FK chain. In Section 2, we recall the formulas for an equilibrium structure, and we argue against using these formulas to apply the twist map. In Section 3, we explain the meaning of the tensile force. In Sections 4 and 5, we discuss the boundary conditions of a finite FK chain and explain with examples the incorrect results of the twist map. Further small points are the energy of the FK chain and the putative problem of the irrational relations of the two periodicities of the FK model. Some aspects of our treatments include connections to an infinite FK chain [21].

2. Equations for Stationary States

At first, it seems that the gap of form (2) does not matter, because for the minimum search for the inner atoms, u_i, holds an equation, where the a_o disappears

$$\frac{\partial U(\mathbf{u})}{\partial u_i} = \frac{2\pi\lambda}{a_s}\sin\Big(\frac{2\,\pi u_i}{a_s}\Big) + k[2\,u_i - u_{i+1} - u_{i-1}] = 0,\ \ i = 2,..,N-1. \tag{3}$$

Note that the linear tensile force with amount μ also disappears [27]. However, the a_o as well as the μ do not disappear at all; they emerge in the two boundary equations for the first and the last atom of the chain, u_1 and u_N [19,28]

$$\frac{\partial U(\mathbf{u})}{\partial u_1} = \frac{2\pi\lambda}{a_s}\sin\Big(\frac{2\,\pi u_1}{a_s}\Big) - k[u_2 - u_1 - a_o] + \mu = 0 \tag{4}$$

and

$$\frac{\partial U(\mathbf{u})}{\partial u_N} = \frac{2\pi\lambda}{a_s}\sin\Big(\frac{2\,\pi u_N}{a_s}\Big) + k[u_N - u_{N-1} - a_o] - \mu = 0\,. \tag{5}$$

Equations (3)–(5), for all atoms $i = 1, \ldots N$, form a system of coupled equations, where we have to include the boundary conditions Equations (4) and (5). To select a single 'solution' of one or a small number of them will usually not give a correct stationary state of the FK chain.

In contrast to this simple remark, many researchers propose to use the 'twist map', which successively calculates one u_{i+1} if the former u_i and u_{i-1} are known—an assumption that we cannot make. If one does not know the solution, one also does not know the location of the two special atoms at the start of the map [19]. In real calculations, the twist map is started at an arbitrary pair of two points in a finite region [21]. Of course, to start the twist map at arbitrary point pairs (see the M_i in Figure 1 of ref. [21]) provides nice pictures, including the excursion to chaos. We claim that many calculations of twist maps do not use the correct initial values; for example, see Example 1 and Section 6 below.

Example 1. *A simple example is a chain with N = 3 atoms, with the parameters* $a_s = 2\,\pi$, $k = 2.5$, $\lambda = 1$, *and* $a_o = 2a_s/3$. *The equilibrium structures of a minimum are obtained by the NMinimize procedure of Mathematica 13.0, starting with a chain with* $u_i = a_o\,(i-1)$ *for* $i = 1,..,3$, *as shown on the left of Figure 1.*

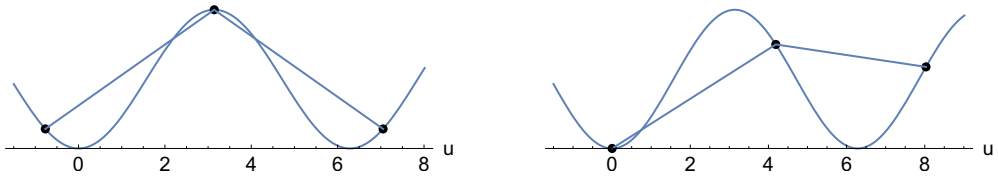

Figure 1. (**Left**): Minimum solution for an FK chain with $N = 3$ atoms. (**Right**): With an arbitrary start of $u_1 = 0$, we obtain $u_2 = a_0 = 2a_s/3$, and we obtain with Equation (3) the shown point u_3. However, the structure is not a minimum, see text. Note that the atoms are shifted on the site-up potential to help the imagination.

Using the twist map of Equations (4) and (3) starting at an arbitrary point, for example, with $u_1 = 0$, we obtain with Equation (4) $u_2 = a_0 = 2a_s/3$, and we obtain with Equation (3) the structure on the right hand side of Figure 1. It does not look like a minimum. The left minimum has an energy of 2.756 units, but this special twist map 'solution' has an energy of 2.826 units. Its gradient $(0, 0, 0.118)^T$ is not a zero vector.

The reason for the deviation of the gradient from zero is that the third Equation (5) for $i = N = 3$ is not fulfilled for the obtained u_3. Only when one begins with u_1 of a stationary structure is the third equation fulfilled. Further arguments to understand the result are given in ref. [19]. We conclude with the following theorem.

Theorem 1. *Using the twist map at an arbitrary start point is useless. In the general case, it will not provide a stationary structure of the FK chain. The reason is that Equation (5) is not fulfilled, in the general case. This is not restricted to the $N = 3$ chain.*

The twist map fulfills the demand of equilibrium only from step to step. Only when the start pair belongs to the correct minimum do the results (under numerical problems, see below) build a correct minimum structure. In the system, one can fulfill some equations—with false values, which vice versa compensate—however, one cannot assume that the other equations obtain the correct solution.

3. A Remark on the Length of the Chain

We treat the energy of the chain structure (1). When the spring distance of the chain, a_o, and the period of the site-up potential, a_s, are equal, and if $\mu = 0$, or if $a_0 = 0$ and $\mu/k = a_s$, or if $a_0 + \mu/k = a_s$, then an equilibrium chain exists in its ground state with all particles at the bottom of the site-up potential, with energy zero for every particle, and thus with zero energy for the chain in its ground state. (This case was originally treated [1] for an infinite chain.)

In any other case, an infinite chain needs an infinite energy in the sum, which is impossible. Strangely, the authors of ref. [29] stated that "...one does not hope that the sum of the energies converges." Nevertheless, they worked with the divergent sum. Tong et al. [30] treated a finite segment of the infinite incommensurate FK chain without the boundary conditions. Without further explanation, the problem was circumscribed by the word 'formal sum' [31,32].

A way out, avoiding the infinite energy of an infinite chain, was proposed [33] by dividing the energy of the chain by N, the number of atoms. So, one has a finite energy per atom [34,35], and one can apply the optimization per atom at u_i, discussed in Section 2 [36].

4. The Meaning of the Tensile Force

If $\lambda = 0$, we see with Equations (4) and (5) that the equilibrium separation of the chain becomes

$$a_0 + \mu/k\,. \tag{6}$$

In addition, if one uses the ansatz of form (2) with $a_0 = 0$, then the value of the tensile force divided by the value of the spring force, μ/k, becomes the placeholder of the a_0 in the original FK model. One can put [37,38]

$$l_o = \mu/k \;\; \rightarrow \;\; \text{new} \;\; a_o \, .$$

The meaning of the tensile force in (2) is to include an equilibrium separation of the chain, l_o for a_0. One can ask why one needs the tensile force.

On the other hand, one can ask for the action of the tensile force, if its amount μ increases. It has the form

$$-\mu \, \mathbf{f}^T \, \mathbf{u}$$

with the special form of the force vector

$$\mathbf{f}^T \; = \; (-1, 0, \ldots, 0, 1) \, .$$

At $\mu = 0$, we may be in an original minimum (with $a_0 = 0$ or not). Increasing the amount of μ, we can optimize another minimum. The curve, which describes the consecutive series of minima, is a Newton trajectory; it was named the curve of the force-displaced stationary points [19,39–44]. Newton trajectories connect stationary points of an index difference of one [45] on the original potential energy surface. It is a quite interesting property that the special form of the **f** vector acts as a change in the orginal distance, a_0, of the atoms of the FK chain, see value (6), and not only as the tilding of the potential of the first and the last atom of the chain. The FK chain is similar to an accordion. If one pulls the ends, all of the bellows relax. Newton trajectories with force **f** can be used to calculate many kinds of solitones of the FK chain and, thus, intermediate minima of the potential energy surface and saddle points with an increasing index [3,6,19,46–48].

5. The Meaning of the Free Boundary Conditions

Now, we discuss the boundary conditions (BCs). If one has free BCs, then we cannot start with an arbitrary 'left' BC, because the minimization will probably result in different BC in the end. So, the steps of an arbitrary twist map start in a nebula. The developments by some researchers [21,49–51] (to name a few), which use the twist map, ignore that the chain will find another minimum structure at the boundary, in comparison to an arbitrary twist map result [19].

Of course, if one starts the twist map with the correct $u_1, \; u_2$ of a minimum structure or of another stationary state of the FK chain, then one can regain this stationary structure with the result of the twist map, at least for the first section of the structure; see the example below. However, we do not know where the stationary structure of an FK chain begins if the BCs are free.

Example 2. *The example is again the chain with parameters* $a_s = 2\pi$, $k = 2.5$, $\lambda = 1$, *and* $a_o = 2a_s/3$, *for* N = 3, 4, 8–10, 20, 47, 74, 99, 500, 1000, *and* $N = 5000$ *atoms. The equilibrium structures, probably minima, are obtained by the NMinimize procedure of Mathematica 13.0 starting with a chain with* $u_i = a_o \, (i-1)$ *for* $i = 1, \ldots, N$. *The first atom of the chain at* u_1 *changes its place with* N, *as well as the average distance*

$$\tilde{a} = \frac{u_N - u_1}{N-1} \, , \tag{7}$$

see Table 1. The numbers in Table 1 are rational numbers, because they are the result of a computer calculation. We do not know whether the character of the limit for N *to* ∞ *is rational or irrational. The two values possibly converge for large* N *against defined values around* $u_1 = 0.369$ *and* a_o. *However, we do not know the exact limit of* $\tilde{a}$.

Table 1. Position of the first atom of a minimum of an FK chain and its average distance.

N	u_1	$\tilde{a}/2\,\pi$	N	u_1	$\tilde{a}/2\,\pi$
3	−0.769	0.6224	47	0.390	0.6700
4	0.117	0.6542	74	0.370	0.6688
8	0.751	0.6801	99	0.358	0.6621
9	−0.341	0.6386	500	0.368	0.6670
10	0.239	0.6582	1000	0.369	0.6665
20	0.632	0.6736	5000	0.369	0.6667

We show in Figure 2 a minimum of an FK chain with $N = 500$ atoms. The central region represents the winding number, the ratio 2/3 of a_o/a_s; however, the two boundary regions show the large influence of the free BCs. A swing in at the left boundary needs ≈50 atoms, and an analogous transient process needs ≈50 atoms at the right boundary. One could imagine that an infinite chain with the 2/3 ratio could be represented by the central piece of Figure 2. However, a cut anywhere relaxes the strain at the border [20], and the shown boundary pattern will emerge again. It also holds for $N = 1000$ and $N = 5000$, where we obtain similar pictures.

The structures of the FK chain at the reported minima are mirror symmetrical up to a length of $N = 46$; see the left panel of Figure 1. Beginning with $N = 47$, the symmetry is broken, and the different form at the two boundaries emerges, as in Figure 2.

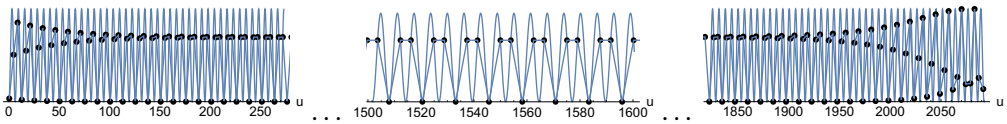

Figure 2. Minimum solution for a fixed a_o, see text. FK chain with $N = 500$ atoms, with the first 66 atoms on the left and the last 66 atoms on the right. The center is an enlarged piece with the regular pattern representing the rational relation to a_s sorting three atoms in two wells.

In Figure 3, we show the corresponding twist map representation of the first 66 atoms for $N = 500$. There, we used the map $\Phi_i = u_i (\mathrm{mod}\ a_s)$ for the minimization result. Consecutive pairs of atoms are shown, (Φ_i, Φ_{i+1}), (Φ_{i+1}, Φ_{i+2}), $(\Phi_{i+2}, \Phi_{i+3}), \ldots$ and so on. The dashed triangle is the start set of points, and the red triangle shows the periodic stable cycle of the central region of the FK chain. The swing in at the left boundary of the chain is the path from the dashed to the red triangle. Note that the points of the inner cycle form a kind of a unit cell defined by the used winding number, 2/3, but they are not free of tension. This is demonstrated by the relaxation at the boundaries.

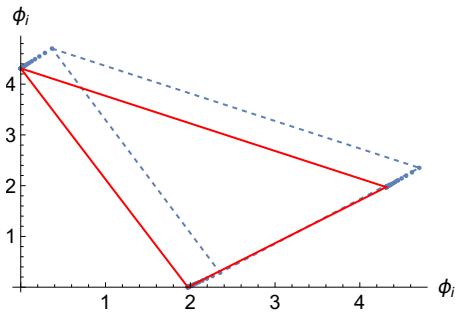

Figure 3. Twist map representation of the first 66 atoms of a long chain. The dashed line is the start triangle of points, and the red line is the quasi-stable cycle of three atoms in one cell of two troughs, as in the central region of Figure 2. (The calculation was a minimization.)

6. The Twist Map for a Finite FK Chain

In the right side of Figure 4, we depict the result of the twist map used with the two correct initial points, $u_1 = 0.369$ and $u_2 = 4.701$, of the optimized structure. The calculation

was performed with Mathematica 13.0 with the usual accuracy. The result fits the true structure up to $N \approx 300$ atoms. Then, the twist map 'breaks out', and at $N = 353$ the former right BC appears. Its way out emerges by numerical effects, which can accumulate over the consecutive iterations.

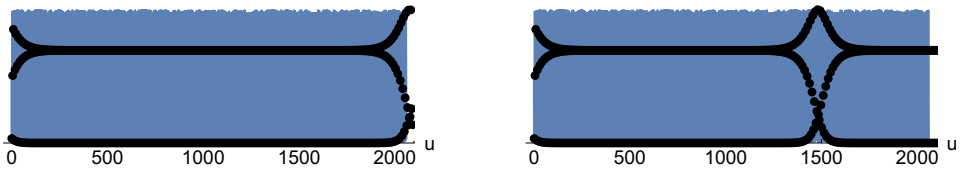

Figure 4. (**Left**): FK chain, optimized minimum with $N = 500$ atoms. (**Right**): The result of the twist map with the two points of the minimum, u_1 and u_2, at the start. It repeats the left BC; however, it 'finishes' at $N = 353$ with a right BC; then, the calculation is reflected.

The twist map must include the handling of the tension of the central quasi-unit cells. The $N = 4$ minimum shown on the left of Figure 5, with a u_1 value of 0.117, is two times 'shorter' than the putative unit cell of $4\pi/3$, see Table 1. The distances of the minimized structure also change from atom to atom in the central part. It only looks like a unit cell. In reality, a unit cell does not exist.

The result for an infinite chain [21] does not hold here, where one has a unit cell if a_o/a_s is a rational number. There is no period of the kind

$$u_{i+3} = u_i + 2\,a_s\,, \quad \text{but it holds} \quad u_{i+3} = u_i + 2\,a_s + \epsilon_i$$

with variable values of ϵ_i. The smallest ϵ_i we find at the central region of the chain with $\epsilon_{244} \approx 2 \times 10^{-11}$.

The fact that even the twist map calculation by Equation (3) finds (though at a false place) a correct upper boundary structure, as the direct optimization does, is very interesting. One has to consider that the quasi-perfect cyclic behavior in the central region is not the behavior of a limit cycle, in contrast to the propositions of ref. [36].

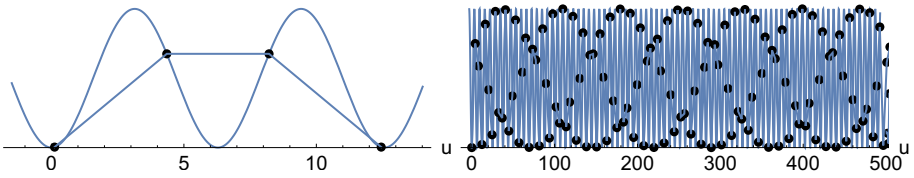

Figure 5. (**Left**): FK chain minimum for $N = 4$ atoms; it is not the unit cell of Figure 2, center; however, it is shorter, see Table 1. (**Right**) The result of a twist map calculation with the two points, $u_1 = 0$ and $u_2 = 2a_s/3$, of a putative unit cell at the start. It does not result in the quasi-unit cells of Figure 2.

Next, we show a twist map calculation in the right panel of Figure 5 and in Figure 6. The start is the putative unit cell with $u_1 = 0$ and $u_2 = 4\,\pi/3$. However, the twist map does not find the structure of consecutive unit cells. It finds that the 3-cycle of Figures 2 and 3 rotates and does not form a correct stable cycle, at least not for three atoms. See the twist map representation in Figure 6.

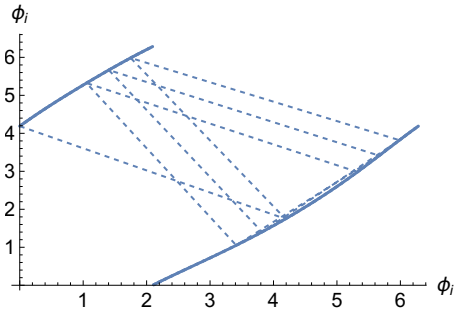

Figure 6. Twist map representation of a twist map calculation with $u_1 = 0$ and $u_2 = 4\pi/3$. The dashed line represents the start sequence of points.

7. The Disappearence of Incommensurabilities

For a given length of a finite FK chain with N atoms for $\lambda = 0$,

$$L_o = (N-1)\, a_o,$$

one can determine an integer M such that the chain of length L_o covers up M troughs of the site potential. If λ is set correctly, the FK chain will fit into the M troughs forming a structure of a minimum with an average separation $\tilde{a}$, with Equation (7). It holds independently of whether the numbers, $L_o, a_o, \tilde{a}$, and a_s, are rational or irrational. One can cite ref. [52] "...a finite chain on a periodic substrate will always be locked because of its free ends." The relation of N to M is in every case a commensurable ratio between two integers [53]; see Example 3.

Example 3. *We treat an example of a chain with a putative 'irrational' winding number [54] of $a_o = 0.873 a_s$ and the other parameters $a_s = 2\pi$, $k = 2.5$, and $\lambda = 1$, for $N = 500$. The equilibrium structure, probably a minimum, is obtained by the NMinimize procedure of Mathematica starting with a chain with $u_i = a_o\,(i-1)$ for $i = 1, \ldots, N$. Figure 7 shows the structure and the corresponding twist map representation.*

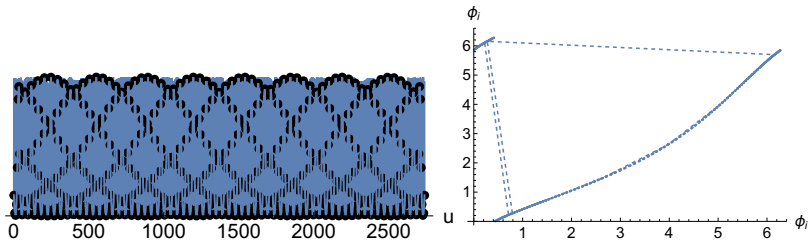

Figure 7. (**Left**): Optimized FK chain minimum for $N = 500$ atoms with winding number 0.873. (**Right**): Twist map representation of the result. The dashed line is the start sequence of nine points plus the first step of the next cycle. It is a quasi-cyclic result.

The structure seems not to be very erratic. The twist map shows a quasi-cycle of nine points. However, the winding number 0.873 is not fully irrational.

8. Remark on the Aubry Transformation of a Finite Chain

There should be a value λ_C, where a qualitative change in the behavior of the infinite FK chain occurs [21,55,56]. For a finite chain, there is no such value. If $\lambda > 0$, and $k > 0$, then the action of the site-up potential will fix the chain in a minimum, if we start a minimization for the 'relaxed' chain with distances a_0; see Section 7.

The putative Aubry-phase transition demonstrated by Figure 6 in ref. [54] is an incorrect interpretation. The first eigenvalue of the second derivatives of the potential of the chain is the frequency for a collective movement of the chain. For an unpinned chain, it has to be zero; thus, the potential has to be flat. However, in the example used in [54], the

first eigenvalue is greater than zero. Thus, the potential is a minimum in both treated cases, $\lambda > \lambda_C$ and $\lambda < \lambda_C$, and the chain is pinned. Of course, the pinning is small if the λ is small. The chain can collectively vibrate; however, it cannot move.

For the interpretation of the experiment [57] with N = 1–5 atoms, we assume that the reported effect is for other reasons.

9. Discussion

We understand the long history of the twist map in the following way:

For a finite FK chain, the parameter a_0 is given; however, the localization of the minimum is unknown. We do not know the values of u_1, u_N, and $\tilde{a}$. Thus, we cannot start the twist map.

To salvage this nevertheless, one assumes a limit l of the average separation and starts with this l anywhere with assumed points u_1 and u_2 for the initial values. One postulates that every arbitrary pair of the start values is possible.

It is clear that the result is not helpful for an original finite FK chain, see Figure 1.

We note that many researchers have treated finite chains [9,33,35,54,57–65] (to name a few); however, they use a useless contrast of rational with irrational numbers in the finite FK model.

In a positive contrast, the treatment in [66] sorts the FK chain in a 'commensurable' way into the site-up potential.

10. Conclusions

We are surprised by researchers' attention to the twist map in the field of the FK model. For a finite FK chain, the twist map theory can only be a supplement; otherwise, important physics conclusions of the model are lost.

Author Contributions: Conceptualization, W.Q. and J.M.B.; software, W.Q.; validation, J.M.B.; writing—original draft preparation, W.Q.; writing—review and editing, J.M.B.; funding acquisition, J.M.B. All authors have read and agreed to the published version of the manuscript.

Funding: This research was funded by the Spanish Ministerio de Economıa y Competitividad, Project No. PID2019-109518GB-I00, and the Spanish Structures of Excellence Maria de Maeztu program through Grant MDM-2017-0767.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: All structure data of FK chains, and Mathematica files are available by e-mail from W.Q.

Conflicts of Interest: The authors declare no conflict of interest.

Abbreviations

The following abbreviations are used in this manuscript:

BC Boundary condition
FK Frenkel–Kontorova

Appendix A

For $k = 0$ and $\mu = 0$, the FK model shortens to the pure site-up potential without spring forces. Any arbitrary distribution of the atoms at the bottom of the siteup potential is possible.

For $\lambda \gg \lambda_c > k > 0$ in the FK model, further minimum structures are possible under $a_0 = 0$, aside from the zero solution discussed in Section 1. λ_c depicts a critical value. Note that every small $k > 0$ prevents the length of the FK chain from becoming too large.

In Figure A1, we depict a case for $N = 8$, $\lambda = 10$, $k = 1$, and $\mu = 0$. The structure has two 'slightly stretched' springs, three 'stretched' springs, and two 'overstretched' springs,

which are possible because of the much smaller k parameter. Note that most of the atoms are not at the minima of the site-up potential, as claimed for large λ [34].

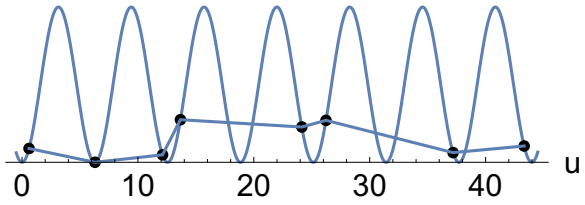

Figure A1. A nonzero FK minimum to potential (2).

References

1. Kontorova, T.A.; Frenkel, Y.I. To the theory of plastic deformations and twinnings I. *Zh. Eksp. Teor. Fis.* **1938**, *8*, 89–95. (In Russian)
2. Lin, J.Y.; Smorodin, A.V.; Badrutdinov, A.O.; Konstantinov, D. Transport Properties of a Quasi-1D Wigner Solid on Liquid Helium Confined in a Microchannel with Periodic Potential. *J. Low Temp. Phys.* **2019**, *195*, 289–299. [CrossRef]
3. Quapp, W.; Lin, J.Y.; Bofill, J.M. The movement of a one-dimensional Wigner solid explained by a modified Frenkel-Kontorova model. *Eur. Phys. J. B* **2020**, *93*, 227. [CrossRef]
4. Duwel, A.E.; Watanabe, S.; Triás, E.; Orlando, T.P.; van der Zant, H.S.J.; Strogatz, S.H. Discreteness-induced resonances and ac voltage amplitudes in long one-dimensional Josephson junction arrays. *J. Appl. Phys.* **1997**, *82*, 4661–4668. [CrossRef]
5. Ustinov, A.V. Solitons in Josephson-junction arrays. *Phys. D* **1998**, *123*, 315–329. [CrossRef]
6. Quapp, W.; Bofill, J.M. Description of Shapiro steps on the potential energy surface of a Frenkel-Kontorova model Part II: Free boundaries. *Eur. Phys. J. B* **2021**, *94*, 64. [CrossRef]
7. Quapp, W.; Bofill, J.M. Description of zero field steps on the potential energy surface of a Frenkel-Kontorova model for annular Josephson junction arrays. *Eur. Phys. J. B* **2021**, *94*, 105. [CrossRef]
8. Grüner, G. The dynamics of charge-density waves. *Rev. Mod. Phys.* **1988**, *60*, 1129–1181. [CrossRef]
9. Garcia-Mata, I.; Zhirov, O.V.; Shepelyansky, D.L. The Frenkel-Kontorova model with cold trapped ions. *Eur. Phys. J. D* **2007**, *41*, 325–330. [CrossRef]
10. Pouget, J.P. The Peierls instability and charge density wave in one-dimensional electronic conductors. *Comptes Rendus Phys.* **2016**, *17*, 332–356. [CrossRef]
11. Braun, O.; Dauxois, T.; Paliy, M.V.; Peyrard, M. Mobility and diffusivity in a generalized Frenkel-Kontorova model. *Phys. Rev. B* **1996**, *54*, 321. [CrossRef]
12. Ekomasov, E.G.; Murtazin, R.R.; Bogomazova, O.B.; Gumerov, A.M. One-dimensional dynamics of domain walls in two-layer ferromagnet structure with different parameters of magnetic anisotropy and exchange. *J. Magn. Magn. Mater.* **2013**, *339*, 133–137. [CrossRef]
13. Trallori, L. Magnetic superlattices, classical spin chains, and the Frenkel-Kontorova model. *Phys. Rev. B* **1998**, *57*, 5923. [CrossRef]
14. Que, W.; Walker, M.B. Generalized Frenkel-Kontorova model for structural modulations in bismuth high-Tc superconductors and related compounds. *Phys. Rev. B* **1992**, *46*, 14772. [CrossRef] [PubMed]
15. Dinsmore, R.C., III; Bae, M.H.; Bezryadin, A. Fractional order Shapiro steps in superconducting nanowires. *Appl. Phys. Lett.* **2008**, *93*, 192505. [CrossRef]
16. Besseling, R.; Niggebrugge, R.; Kes, P.H. Transport properties of vortices in easy flow channels: A Frenkel-Kontorova study. *Phys. Rev. Lett.* **1999**, *82*, 3144–3147. [CrossRef]
17. Kokubo, N.; Besseling, R.; Vinokur, V.M.; Kes, P.H. Mode Locking of Vortex Matter Driven through Mesoscopic Channels. *Phys. Rev. Lett.* **2002**, *88*, 247004. [CrossRef]
18. Iaroshenko, O.; Rybalko, V.; Vinokur, V.M.; Berlyand, L. Vortex phase separation in mesoscopic superconductors. *Sci. Rep.* **2013**, *3*, 1758. [CrossRef]
19. Quapp, W.; Bofill, J.M. Newton Trajectories for the Frenkel-Kontorova model. *Mol. Phys.* **2019**, *117*, 1541–1558. [CrossRef]
20. Kochendörfer, A.; Seeger, A. Theorie der Versetzungen in eindimensionalen Atomreihen. I. Periodisch angeordnete Versetzungen. *Zeitschr. Phys.* **1950**, *127*, 533–550. [CrossRef]
21. Aubry, S. The twist map, the extended Frenkel-Kontorova model and the devil's staircase. *Phys. D* **1983**, *7*, 240–258. [CrossRef]
22. Hobart, R.; Celli, V. A Solution to the Frenkel-Kontorova Dislocation Model. *J. Appl. Phys.* **1962**, *33*, 60–62. [CrossRef]
23. Hu, B.; Shi, J. Nonanalytic twist maps and Frenkel-Kontorova models. *Phys. D* **1994**, *71*, 23–38. [CrossRef]
24. Aubry, S. Defectibility and frustration in incommensurate structures: The devil's stair case transformation. *Ferroelectrics* **1980**, *24*, 53–60. [CrossRef]
25. Guo, Y.; Qu, Z.; Zhang, Z. Lyapunov stability and precise control of the frictional dynamics of a one-dimensional particle array. *Phys. Rev. B* **2006**, *73*, 094118. [CrossRef]
26. Theodorakopoulos, N.; Peyrard, M.; MacKay, R.S. Nonlinear Structures and Thermodynamic Instabilities in a One-Dimensional Lattice System. *Phys. Rev. Lett.* **2004**, *93*, 258101. [CrossRef]
27. Aubry, S. Devils staircase and order without periodicity in classical condensed matter. *J. Phys. Fr.* **1983**, *44*, 147–162. [CrossRef]

28. Frank, F.C.; van der Merwe, J.H. One-Dimensional Dislocations. I. Static Theory. *Proc. R. Soc. Lond. A* **1949**, *198*, 205–216.
29. Blass, T.; de la Llave, R. The Analyticity Breakdown for Frenkel-Kontorova Models in Quasi-periodic Media: Numerical Explorations. *J. Stat. Phys.* **2013**, *150*, 1183–1200. [CrossRef]
30. Tong, P.; Li, B.; Hu, B. Wave transmission, phonon localization, and heat conduction of a one-dimensional Frenkel-Kontorova chain. *Phys. Rev. B* **1999**, *59*, 8639. [CrossRef]
31. Aubry, S.; MacKay, R.S.; Baesens, C. Equivalence of uniform hyperbolicity for symplectic twist maps and phonon gap for Frenkel-Kontorova models. *Phys. D* **1992**, *56*, 123–134. [CrossRef]
32. Salahshoor, H.; de la Llave, R. A Numerical Investigation of the Pinning Phenomenon in Quasi-Periodic Frenkel-Kontorova Model Under an External Force. *J. Stat. Phys.* **2018**, *173*, 398–410. [CrossRef]
33. Hu, B.; Li, B.; Zhao, H. Mode-locking of incommensurate phase by quantum zero point energy in the Frenkel-Kontorova model. *Europhys. Lett.* **2001**, *53*, 342. [CrossRef]
34. Griffiths, R.B.; Chou, W. Effective Potentials: A New Approach and New Results for One-Dimensional Systems with Competing Length Scales. *Phys. Rev. Lett.* **1986**, *56*, 1929. [CrossRef] [PubMed]
35. Sharma, S.R.; Bergersen, B.; Joos, B. Aubry transition in a finite modulated chain. *Phys. Rev. B* **1984**, *29*, 6335–6340. [CrossRef]
36. Baesens, C.; MacKay, R.S. Gradient dynamics of tilted Frenkel-Kontorova models. *Nonlinearity* **1998**, *11*, 949–964. [CrossRef]
37. Aubry, S.; Abramovici, G. Chaotic trajectories in the standard map. The concept of anti-intergability. *Phys. D* **1990**, *43*, 199–219. [CrossRef]
38. Aubry, S.; Le Daeron, P.Y. The diskrete Frenkel-Kontorova model and its extensions I. Exact results for the ground-states. *Phys. D* **1983**, *8*, 381. [CrossRef]
39. Avdoshenko, S.M.; Makarov, D.E. Reaction Coordinates and Pathways of Mechanochemical Transformations. *J. Phys. Chem. B* **2015**, *120*, 1537–1545. [CrossRef]
40. Bofill, J.M.; Ribas-Ariño, J.; García, S.P.; Quapp, W. An Algorithm to Locate Optimal Bond Breaking Points on a Potential Energy Surface. *J. Chem. Phys.* **2017**, *147*, 152710. [CrossRef]
41. Quapp, W. Can We Understand the Branching of Reaction Valleys for more than two Degrees of Freedom? *J. Math. Chem.* **2015**, *54*, 137–148. [CrossRef]
42. Quapp, W.; Bofill, J.M. A contribution to a theory of mechanochemical pathways by means of Newton trajectories. *Theor. Chem. Acc.* **2016**, *135*, 113. [CrossRef]
43. Quapp, W.; Bofill, J.M. Mechanochemistry on the Müller-Brown Surface by Newton Trajectories. *Int. J. Quant. Chem.* **2018**, *118*, e25522. [CrossRef]
44. Quapp, W.; Bofill, J.M.; Ribas-Ariño, J. Towards a Theory of Mechanochemistry, Simple Models from the Very Beginnings. *Int. J. Quant. Chem.* **2018**, *118*, e25775. [CrossRef]
45. Hirsch, M.; Quapp, W. Reaction Channels of the Potential Energy Surface: Application of Newton Trajectories. *J. Mol. Struct. Theochem* **2004**, *683*, 1–13. [CrossRef]
46. Quapp, W.; Bofill, J.M. A Model for a Driven Frenkel-Kontorova Chain. *Eur. Phys. J. B* **2019**, *92*, 95–117. [CrossRef]
47. Quapp, W.; Bofill, J.M. Sliding Paths for Series of Frenkel-Kontorova Models—A Contribution to the Concept of 1D-superlubricity. *Eur. Phys. J. B* **2019**, *92*, 193. [CrossRef]
48. Quapp, W.; Bofill, J.M. Description of Shapiro steps on the potential energy surface of a Frenkel-Kontorova model Part I: Chain in a box. *Eur. Phys. J. B* **2021**, *94*, 66. [CrossRef]
49. Bichoutskaia, E.; Heggie, M.I.; Lozovik, Y.E.; Popov, A.M. Multi-Walled Nanotubes: Commensurate-Incommensurate Phase Transition and NEMS Applications. *Fuller. Nanotubes Carbon Nanostruct.* **2006**, *14*, 131–140. [CrossRef]
50. Black, R.C.; Satija, I.I. Universal phase diagram in the generalized Frenkel-Kontorova model. *Phys. Rev. B* **1991**, *44*, 4089–4096. [CrossRef]
51. Vanossi, A.; Bechinger, C.; Urbakh, M. Structural lubricity in soft and hard matter systems. *Nat. Commun.* **2020**, *11*, 4657. [CrossRef] [PubMed]
52. Stoyanov, S.; Müller-Krumbhaar, H. Resonance-induced Cluster-mobility: Dynemics of a finite Frenkel-Kontorova model. *Surf. Sci.* **1985**, *159*, 49–68. [CrossRef]
53. Quapp, W.; Bofill, J.M. Comment on 'Out-of-equilibrium Frenkel-Kontorova model' (A. Imparato, 2021, J. Stat. Mech. 013214). *J. Stat. Mech.* **2022**, *2022*, 013204. [CrossRef]
54. Muñoz, J.M.; Sawant, R.; Maffei, A.; Wang, X.; Barontini, G. Realizing the Frenkel-Kontorova model with Rydberg-dressed atoms. *Phys. Rev. A* **2020**, *102*, 043308. [CrossRef]
55. Axel, F.; Aubry, S. Polarisation and transition by breaking of analyticity in a one-dimensional model for incommensurate structures in an electric field. *J. Phys. A* **1987**, *20*, 487. [CrossRef]
56. Peyrard, M.; Aubry, S. Critical behaviour at the transition by breaking of analyticity in the discrete Frenkel-Kontorova model. *J. Phys. C Solid State Phys.* **1983**, *16*, 1593–1608. [CrossRef]
57. Bylinskii, A.; Gangloff, D.; Counts, I.; Vuletić, V. Observation of Aubry-type transition in finite atom chains via friction. *Nat. Mater.* **2016**, *15*, 717–721. [CrossRef]
58. Babushkin, A.Y.; Abkaryan, A.K.; Dobronets, B.S.; Krasikov, V.S.; Filonov, A.N. The Ground State of the Frenkel-Kontorova Model. *Phys. Solid State* **2016**, *58*, 1834–1845. [CrossRef]
59. Ma, Y.; Wang, J.; Xu, X.; Wei, Q.; Kais, S. A density-matrix renormalization group Study of one-dimensional incommensurate quantum Frenkel-Kontorova model. *J. Phys. Soc. Jpn.* **2014**, *83*, 094605. [CrossRef]

60. Mikheikin, I.D.; Kuznetsov, M.Y.; Makhonina, E.V.; Pervov, V.S. Defects in Inorganic Suprastructures with Incommensurate Structural Elements: The Static Frenkel-Kontorova Model for Finite Systems. *Dokl. Phys. Chem.* **2001**, *376*, 52–55. [CrossRef]
61. Nasilowski, R. An unorthodox analysis of the Frenkel-Kontorova model. *Phys. A* **1996**, *230*, 266–284. [CrossRef]
62. Novak, I.; Truskinovsky, L. Segmentation in cohesive systems constrained by elastic environments. *Phil. Trans. R. Soc. A* **2017**, *375*, 20160160. [CrossRef] [PubMed]
63. Wang, C.L.; Tekić, J.; Duan, W.S.; Shao, Z.G.; Yang, L.P. Existence and stability of the resonant phenomena in the dc- and ac-driven overdamped Frenkel-Kontorova model with the incommensurate structure. *Phys. Rev. E* **2011**, *84*, 046603. [CrossRef] [PubMed]
64. Zhirov, O.V.; Lages, J.; Shepelyansky, D.L. Thermoelectricity of cold ions in optical lattices. *Eur. Phys. J. D* **2019**, *73*, 149. [CrossRef]
65. Zhirov, O.V.; Lages, J.; Shepelyansky, D.L. Thermoelectricity Modeling with Cold Dipole Atoms in Aubry Phase of Optical Lattice. *Appl. Sci.* **2020**, *10*, 2090. [CrossRef]
66. Thomas, A.; Leoni, T.; Siri, O.; Becker, C.; Unzog, M.; Kern, C.; Puschnig, P.; Zeppenfeld, P. A one-dimensional high-order commensurate phase of tilted molecules. *Phys. Chem. Chem. Phys.* **2022**, *24*, 9118. [CrossRef] [PubMed]