LETTER

On putative incommensurate states of a finite Frenkel-Kontorova chain

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We propose a new but simpler explanation of the phases of a Frenkel-Kontorova chain of atoms, and we demonstrate it by examples. Combined with this, we present a criticism of the theory of so-called commensurate and incommensurate states, especially for finite chains. We reject the putative observation of an Aubry-phase transition in a finite chain.

Keywords: Frenkel-Kontorova model, Phase, Average particle-particle distance

I. INTRODUCTION

This letter is devoted to the aim of understanding what happens inside the finite Frenkel-Kontorova (FK) chain[1–3], if the two characteristic ratios a/b and V_o/k change. We select ref. 4 to discuss some general problems of the understanding of the FK model, with the special example of this paper. For shortness we only treat the springlike potential of ref. 4.

The corresponding model of the potential energy of a linear FK chain $\mathbf{x} = (x_1, ..., x_N)$ with $x_i < x_{i+1}$ for all atoms, and with atoms of equal mass at points x_i is [4]

$$U(\mathbf{x}) = V_o \sum_{i=1}^{N} (1 - cos(\frac{2\pi}{b} x_i)) + \frac{k}{2} \sum_{i=1}^{N-1} V_{int}(x_{i+1} - x_i) . \tag{1}$$

V_o describes the strongness of the substrate but k describes the strongness of the springlike forces between neighboring atoms. Used are $V_o = 0.02, k/k_B = 783.6$ (without units[4]). Parameter b is the periodicity of the substrate. It is used with a variable length around the spring distance of the V_{int} potential, $a = 2.4$. This interatomic springlike potential function is

$$V_{int}(r) = \frac{-1}{1 + c_o(r - r_o)^2} + \frac{1}{k} Exp(-c_2(r - r'_o)) . \tag{2}$$

The following parameters of the function are used[4] c_o=12.9, r_o=2.4, c_2=263.0, r'_o=1.8.

The graph of function (2) is shown in Fig.1. The minimum is found to be at $a = r_{min} = 2.4$ units, in contrast to ref. 4 with 2.44 units. We used the Mathematica program, version 13.0, for the calculations, as well as for the Figures.

The springlike potential is of special interest because it is unsymmetrical for stretching against compression.
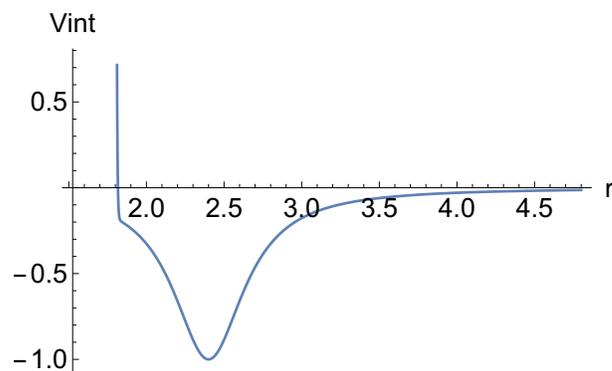
FIG. 1. The springlike potential function of Eq.(2).

However for the calculation of minima this fact alone does not play a role. The boundary conditions for x_1 and x_N are free. Parameter $a = r_{min}$ is the distance of two atoms if the parameter V_o is zero. It is hold fixed throughout the letter. However, in the chain with the substrate potential, $V_o \neq 0$, usually the average distance, $\tilde{a}$, changes to

$$\tilde{a} = \frac{x_N - x_1}{N - 1} , \tag{3}$$

because the chain will find a minimum form in the substrate[5], compare Fig.2. We have to emphasize that $\tilde{a}$ is the average distance in a minimum structure.

In our calculations on the relation of the influence of the two parts of Eq.(1) we only change the parameters b, V_o of the substrate potential. The spring potential and k are fixed.

II. COMMENSURATE MINIMA

Our remark concerns the discussion of commensurate or incommensurate states of the chain. Note that this letter is similar to another one[6]. Thus, the problem may be widespread distributed in the FK community.
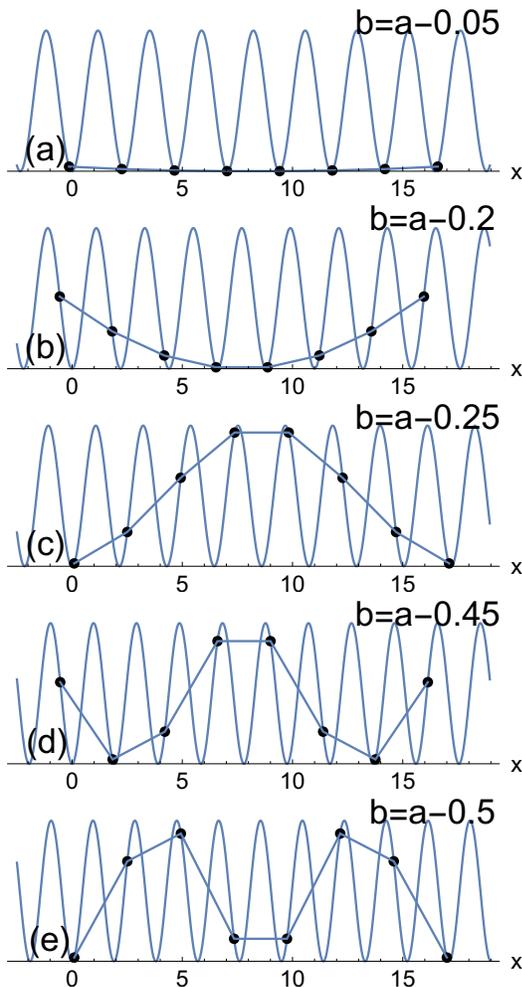
FIG. 2. Ground state of FK chains of different b values. Only the substrate potential is shown, however, the fixed springlike force is not shown. To lead the eye, we moved the atoms up to the potential line. Note the different length of the substrate throughs. In (c) and in (e) new kinks emerge. The outer atoms show impressively the effect of the free boundaries.

We start with the chain at the potential energy (1). We determine the minimizer of the chain in the combined two potentials (1), by the substrate and by the springlike forces. The definition of a 'commensurate' chain in ref. 4 is useless, because it is empty if $Q > N$

$$x_{Q+i} = x_i + R\,b \qquad (4)$$

for integers Q, R. Then x_{Q+i} would be outside the chain. For example it is the case for $N = 50$ and $R/Q = 52/51$. Note that cases $Q > N$ will come far before an irrational relation of $\tilde{a}/b$. Of course, for nearly all cases with $a \neq b$ we will find some atoms at x_i outside the bottom of their corresponding through.

We have recalculated a part of a similar curve like in Fig.4, part (a-3)[4]. A result is shown in our Fig. 2 by some special chains belonging to the case $V_0 = 0.9\,k$. Calculations are executed for steps $b = a - s * 0.05$ for the

step numbers $s = 0, .., 10$ in the $[a - 0.5, a]$ interval for b. The springlike potential with parameter a is not changed. In every case, we 'sort' the constantly equal chain into different substrate throughs. And there it changes, see Fig. 2.

To see what happens in the FK chain, we only used $N = 8$ atoms (and not 50 like it is done in ref. 4). We always start the minimization of the chain with $x_1 = 0$ and $x_i = a\,(i - 1)$ for $i = 2, ..., N$. We get steps like in Fig.4 of ref. 4. Of course, only rational numbers are used for the steps. The step near the line 1 is not constant; it slowly increases to the right hand side.

We conclude that the statement that there are "small intervals of zero slope"[4,7] is not correct. The increase comes from a small ascent of the $\approx N/2$ left atoms to the left walls of their corresponding substrate potential throughs, and of the $\approx N/2$ right atoms to the right walls of their corresponding substrate throughs, what increases $\tilde{a}$. This implies that this fact does not have relations with commensurate, or incommensurate numbers.

We explain the steps in Fig.2. It is $\tilde{a} = 2.39$, 2.36, 2.25, 2.38, and 2.38 correspondingly, and $\tilde{a}/b$ is then 1.02, 1.07, 1.13, 1.22 and 1.25. Thus we really get consecutive states on the staircase like in Fig.4 of ref. 4.

The step from part (a) to (b) for a shorter b, thus a larger a/b, shows a climbing up of the outer atoms to their left walls (the $N/2$ left ones) or to the right hand side walls (the right $N/2$ atoms) .

Between (b) and (c) happens a 'phase' jump, see below a definition of a phase. Now the chain occupies one through more of the substrate, not $N = 8$ however 9 waves. This is possible because the central through, say with number 5, is now empty. The chain has a kink. Note that all structures in Fig.2 are minima.

Part (d) is again a stretching of the chain, but a/b correctly increases.

A next 'phase' jump happens between (d) and (e). Again a new kink emerges. Now two kinks concern the throughs 3 and 8 of the substrate, which are bridged by the kinks.

The key is that one or two atoms, x_5 in (c), or x_3 and x_8 in part (e), jump at the end of the increasing movement over a peak of the site-up potential. Note that the new kinks are not restricted to the center of the chain, as it has been claimed in a former work[8]. The pattern of new kinks repeats for higher values of a/b again and again at every step. So the jumps emerge in Fig.4 of ref. 4. Thus, the given jumps are correct.

The pure minima of the FK-chain with $N = 8$ atoms disclose 3 'phases' in the region $1 \leq a/b \leq 1.265$. The minimization of Mathematica leads to the same phase for certain intervals of a/b. The character of the used number b rational or irrational, is irrelevant. What counts is the length of the chain, given by the a, and the (integer) number of throughs of the substrate, which the chain occupies. Any distinction into commensurate or incommensurate is nonsense here.

From Cantor's proof that the real numbers are un-

countable but the rational numbers are countable, it follows that almost all real numbers are irrational. But the rational numbers are dense as well as the irrational ones. There is no gap in both kinds of numbers which indicates the steps in Fig.4 of ref.[4]

The statement of ref. [4] that "the ratio a/b is highly irrational and quite far from a rational value" is not correct. There is no smallest distance from every irrational number to any "neighboring" rational one. If z is irrational, and if such a distance existed then we coud take the "left" rational number z_1 and the "right" rational number z_2 and build the rational number $(z_1 + z_2)/2$ which is nearer to the initial z number.

We conclude that relating 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. And we wonder how the authors of ref. [4] have decided the different kind of results in their Fig.4 to be 'rational' or 'irrational' steps? We have to assume that they used a computer for their calculation. Every numerical calculation on a computer goes on with a (restricted) range of rational numbers. Irrational numbers are not representable. We cannot imagine how they use an irrational b, and we cannot imagine how they know that the result $\tilde{a}$ is 'irrational'.

The adsorption of the chain by the substrate acts in the way 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. Every limit $N \to \infty$ is a mathematical abstraction. Nowhere in ref. [4] we could find a treatment of such a limit process.

Thus one can assume that to every constellation of the parameters a/b, V_o/k, and N, exits at least one minimizer, a structure of the FK chain in a minimum of the combined potential (1). We now explicitly define different 'phases' of the chain.

III. DEFINITION OF A PHASE

If an equilibrium structure of the FK chain occupies L throughs 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 the the same phase.
A single phase transition is correspondingly a change of an equilibrium structure of the FK-chain to $L + 1$ or $L - 1$ throughs. (We have outlined above that the "commensurate-definition" by Eq. (4) may be empty.) 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 throughs. This is connected by a jump in the average $\tilde{a}$, see Fig. 2. The question circles around the count of integers.

Besides the ratio of a/b the balance of k and V_o also plays a role. In all cases, the chains like in Fig. 2 are regular structures, no kind of incommensurability

emerges at any a/b as it is claimed in ref. [4].

We still treat the case $N \to \infty$. In ref. [4] is treated the finite case only, for $N = 50$. We find that the larger N is, the 'earlier' a small change in parameter b leads to a change of the number of occupied throughs. Because the unperturbed chain ends at $x_N = (N - 1)\,a$. If then b is so much smaller that holds

$$N\,b\ < (N - 1)\,a$$

then the minimization leads to a kink. It means a step in the 'staircase'. However, in the condition

$$a > \frac{N}{N - 1}\,b \tag{5}$$

the factor at b converges to 1 in N for every finite V_o and k. However, for larger and larger N, thus the limit treatment, formula (5) leads to the decrease of the step length of the staircase of Fig. 4 in ref. [4] to zero. The staircase of Fig. 4 in ref. [4] degrades to a straight line. Any kind of "devils staircase"[4,7] disappears in the limit.

IV. PHASE CHANGES

A next section concerns the putative Aubry-phase transition demonstrated by Fig. 6 in ref.[4] 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, here the first eigenvalue is greater than zero, for the blue points, as well as for the red points of Fig. 6 in ref.[4]. Thus the potential is a minimum, in both cases, and the chain is pinned. Of course, the pinning is small if the V_o is small. The chain can collectively vibrate, however it cannot move. The step in the higher eigenvalues under the red points concerns inner vibrations of the chain. This has nothing to do with pinned or unpinned states. Unpinned versions of a ground state of a finite FK chain are not correctly calculated. (If V_o is not zero. And if V_o is zero then we do not have the FK model, at all.)

V. DISCUSSION

We ask for the fascination of irrationals for workers in the field of the FK model. The early source may be the papers of S.Aubry[9–14]. Our main contradiction to these works is the use of an infinite chain. For any 'limit'-process which one needs to treat such a chain, the correct way would be to study a finite chain with N particles, to determine its equilibrium structure, and then to increase step by step the number, N, of the chain, more and more up to a limit. However, such a treatment is missing in the papers of S.Aubry.

Note, an actual infinity is not possible, as well as an infinite long chain. Such a construct does not exist in

reality. In Mathematics only one studies the possibility of infinite rows, for example, and their convergence, or divergence. There are strong rules for the handling of the 'infinity'.

Especially, we miss the treatment of the boundary conditions (BCs), over which the distance of the chains spring, $a = r_{min}$, (see Fig. 1) comes into play. Without the BCs this parameter of the chain disappears in many FK studies. This is questionable. If one has free BCs then we cannot start with a fixed 'left' BC because the minimization will result finally in a probably other BC. So all the steps of the twist map start in a nebula. The development by S.Aubry[15], and others[16–18] which use the twist map, ignores that the chain will find at the boundary another minimum structure, in comparison to any twist map result[3]. If there are assumed fixed BCs, for example, and one starts 'left' with the left BC, and one uses all the steps throughout the twist map then usually the result at the 'right' end of the chain will not fit the right BC. (However, nobody can put BCs at infinity, and nobody can really start at minus infinite, at all.)

We still note that some workers reduce their treatment[19–27] (to name a few) to finite chains, what is quite correct, however, they continue using the erroneous contrast of rational to irrational numbers in the finite FK model.

In a positive contrast, there is a treatment[28] which sorts the FK chain in a 'commensurable' kind into the site-up potential.

VI. CONCLUSION

This letter discusses the widespread theory of so-called commensurate (C) versus incommensurate (IC) phases of the FK model[4,7]. We have seen that the C-phases 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 find no broken regular arrangement of the atoms of the chain, either. 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.

In a 2D or 3D crystal lattice a long-range periodic order with an irrational ratio of the periodicities[7,29] can exist. Its description as an IC crystal is in order. However, the $\tilde{a}$ in the FK model is not the description of a fixed lattice. It is 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 basins 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 or stretches to another number of basins of the site-up potential, has nothing to do with

rational or irrational numbers.

As discussed above, one of the origins of the incorrect 'C-IC sight' may be due to the theory of S. Aubry. There is already an analysis of this non-appropriete theory[3,6].

REFERENCES

[1]T. A. Kontorova and Y. I. Frenkel, "To the theory of plastic deformations and twinnings I (in russian)," Zh. Eksp. Teor. Fis. **8**, 89–95 (1938).

[2]T. A. Kontorova and Y. I. Frenkel, "To the theory of plastic deformations and twinnings II (in russian)," Zh. Eksp. Teor. Fis. **8**, 1340–1348 (1938).

[3]W. Quapp and J. M. Bofill, "Newton trajectories for the Frenkel-Kontorova model," Molec. Phys. **117**, 1541–1558 (2019).

[4]J. M. Muñoz, R. Sawant, A. Maffei, X. Wang, and G. Barontini, "Realizing the Frenkel-Kontorova model with Rydberg-dressed atoms," Phys. Rev. A **102**, 043308 (2020).

[5]S. Stoyanov and H. Müller-Krumbhaar, "Resonance-induced cluster-mobility: Dynemics of a finite Frenkel-Kontorova model," Surface Sci. **159**, 49–68 (1985).

[6]W. Quapp and J. M. Bofill, "Comment on 'Out-of-equilibrium Frenkel-Kontorova model' (A. Imparato, 2021, J. Stat. Mech. 013214)," J. Stat. Mech. , 013204 (2022).

[7]P. M. Chaikin and T. C. Lubensky, *Principles of Condensed Matter Physics* (Cambridge University Press, Cambridge, 1995).

[8]I. D. Mikheikin, M. Y. Kuznetsov, E. V. Makhonina, and V. S. Pervov, "The Frenkel-Kontorova model for studying suprastructures with incommensurate elements," J. Mat. Syn. Proc. **10**, 53–60 (2002).

[9]S. Aubry, "The twist map, the extended Frenkel-Kontorova model and the devils staircase," Physica **7D**, 240–258 (1983).

[10]M. Peyrard and S. Aubry, "Critical behaviour at the transition by breaking of analyticity in the discrete Frenkel-Kontorova model," J. Phys. C: Solid State Phys. **16**, 1593–1608 (1983).

[11]S. Aubry, "Devils staircase and order without periodicity in classical condensed matter," J. Phys. France **44**, 147–162 (1983).

[12]S. Aubry and P. Y. Le Daeron, "The discrete Frenkel-Kontorova model and its extensions I. Exact results for the ground-states," Physica D **8**, 381 (1983).

[13]F. Axel and S. Aubry, "Polarisation and transition by breaking of analyticity in a one-dimensional model for incommensurate structures in an electric field," J. Phys. A **20**, 487 (1987).

[14]M. Johansson, G. Kopidakis, S. Lepri, and S. Aubry, "Transmission thresholds in time-periodically driven nonlinear disordered systems," Europhys. Lett. **86**, 10009 (2009).

[15]S. Aubry, "Equivalence of uniform hyperbolicity for symplectic twist maps and phonon gap for Frenkel-Kontorova models," Phys. D **56**, 123–134 (1992).

[16]R. C. Black and I. I. Satija, "Universal phase diagram in the generalized Frenkel-Kontorova model," Phys. Rev. B **44**, 4089–4096 (1991).

[17]E. Bichoutskaia, M. I. Heggie, Y. E. Lozovik, and A. M. Popov, "Multi-walled nanotubes: Commensurate-incommensurate phase transition and NEMS applications," Fullerenes, Nanotubes, Carbon Nanostructures **14**, 131–140 (2006).

[18]A. Vanossi, C. Bechinger, and M. Urbakh, "Structural lubricity in soft and hard matter systems," Nat. Comm. **11**, 4657 (2020).

[19] S. R. Sharma, B. Bergersen, and B. Joos, "Aubry transition in a finite modulated chain," Phys. Rev. B **29**, 6335 – 6340 (1984).

[20] B. Hu, B. Li, and H. Zhao, "Mode-locking of incommensurate phase by quantum zero point energy in the Frenkel-Kontorova model," Europhys. Lett. **53**, 342 (2001).

[21] I. D. Mikheikin, M. Y. Kuznetsov, E. V. Makhonina, and V. S. Pervov, "Defects in inorganic suprastructures with incommensurate structural elements: The static Frenkel-Kontorova model for finite systems," Dokl. Phys. Chem. **376**, 52–55 (2001).

[22] I. Garcia-Mata, O. V. Zhirov, and D. L. Shepelyansky, "The Frenkel-Kontorova model with cold trapped ions," Eur. Phys. J. D **41**, 325–330 (2007).

[23] C. L. Wang, J. Tekić, W. S. Duan, Z. G. Shao, and L. P. Yang, "Existence and stability of the resonant phenomena in the dc- and ac-driven overdamped Frenkel-Kontorova model with the incommensurate structure," Phys. Rev. E **84**, 046603 (2011).

[24] Y. Ma, J. Wang, X. Xu, Q. Wei, and S. Kais, "A density-matrix renormalization group study of one-dimensional incommensurate quantum Frenkel-Kontorova model," J. Phys. Soc. Jpn. **83**, 094605 (2014).

[25] A. Bylinskii, D. Gangloff, I. Counts, and V. Vuletić, "Observation of Aubry-type transition in finite atom chains via friction," Nature Materials **15**, 717–721 (2016).

[26] A. Y. Babushkin, A. K. Abkaryan, B. S. Dobronets, V. S. Krasikov, and A. N. Filonov, "The ground state of the Frenkel-Kontorova model," Phys. Solid State **58**, 1834 – 1845 (2016).

[27] I. Novak and L. Truskinovsky, "Segmentation in cohesive systems constrained by elastic environments," Phil. Trans. R. Soc. A **375**, 20160160 (2017).

[28] A. Thomas, T. Leoni, O. Siri, C. Becker, M. Unzog, C. Kern, P. Puschnig, and P. Zeppenfeld, "A one-dimensional high-order commensurate phase of tilted molecules," Phys. Chem. Chem. Phys. **24**, 9118 (2022).

[29] V. S. Pervov and E. V. Makhonina, "Incommensurate suprastructures: new problems of inorganic solid-state chemistry," Russ. Chem. Rev. **69**, 481–489 (2000).