



The Frenkel-Kontorova Model – A never ending Tale –

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Abstract

The Frenkel-Kontorova (FK) model is a physical model, which can be imagined as a chain of pendulums, which are coupled to each other. It successfully describes dislocations in solids or in crystals and other phenomena, thus it is applied in many ways in solid state physics. By various additional assumptions or modifications of the original approach it results in an extended theory, which is still being studied today. Here mainly stationary states of the simplest model shall be discussed, which give rise to the notion of a soliton.

Additionally a transition from the discrete to the continuous form, of the chain of oscillators to a vibrating string with nonlinear excitation, is treated. The latter moves according to the so-called Sine-Gordon equation, a well-known soliton equation. A soliton solution describes, among other things, a long-lived wandering disorder in a crystal.

In another limit transition, a supposed extension of the chain to infinity is criticized, and wrong uses of the so-called twist map are revealed.

Keywords

FK Model, Soliton, Newton Trajectory, Potential Energy Surface, Sine-Gordon Equation, Twist Map

1 Introduction

This review is the slightly expanded ‘paper form’ of a talk given at the Leibniz-Sozietät zu Berlin in February 2023¹ (in German language).

The following points are covered in this review:

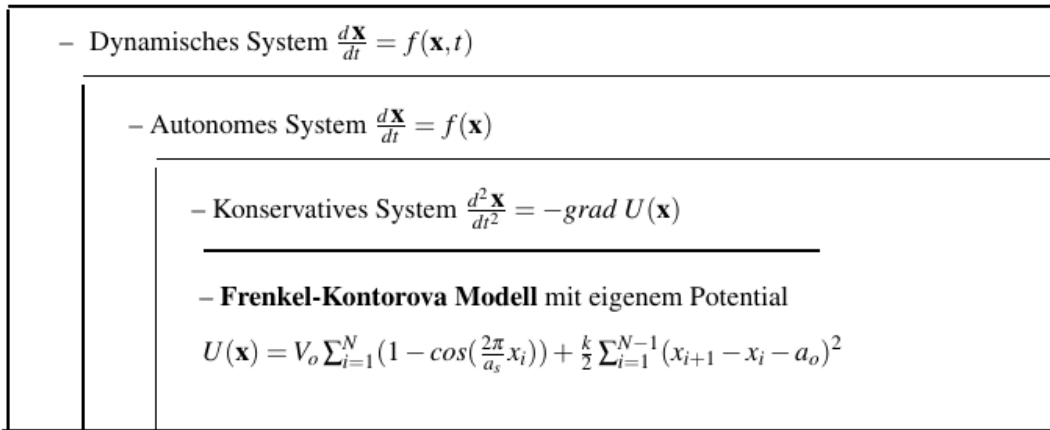
- The basic concepts in which the FK model is embedded.
- The FK model itself is introduced, important are: same or different periodicity of the two potentials,
- minima as ground states and high lying intermediaries as well as transitions over saddle points.
- Properties of excited states will lead us to the notion of a **soliton**.
- Important applications will be mentioned – examples presented.
- In a second part, two limit processes will be discussed:
- Once the FK model and the vibrating string,
- and the dubious transition to an infinitely ‘long’ chain. We polemicize here against the misapplication of the twist map.

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Basic concepts

The theory of **dynamic systems** models motion or evolution, how a **state** \mathbf{x} changes in the course of time t . If the process is homogeneous with respect to time, i.e. it depends only on the initial state, but not on the choice of the initial time, then it is called an autonomous system. The time t can be discrete (integer) or continuous. The space of states \mathbf{x} has a dimension N , i.e. \mathbf{x} is a vector. One writes $\mathbf{x}=(x_1, x_2, \dots, x_N)^T$. Important questions in dynamic systems concern their long-term behavior (for example, stability, periodicity, chaos, and ergodicity) and their control.

Scheme 1: The FK model fits into the following systems of differential equations



Mainly stationary states of the FK potential will be considered in this summary. The second order dynamic equation is used at the limit transition to the sine-Gordon equation.



2 The FK Model

The model was introduced by Yakov Il'itch FRENKEL (1894 - 1952), Prof. for Theoretical Physics at University Leningrad, and

Tatjana Abramovna KONTOROVA (1911 - 1976). She was the assistant of Frenkel. She submitted a dissertation on the mechanics of plastic deformation of crystals (1938), from which this model originated. Further works by her exist on intercrystalline layers, on catalysts, solid-state physics, semiconductors, and on studies of Germanium.

The **original works** to 'Frenkel-Kontorova-Model' were given in 1938/1939.²⁻⁶

Yakov Il'itch FRENKEL was born on 10.2.1894, Rostov-am-Don.

1913-1916 he studied at the University of St. Petersburg, after that he was there a research associate, later professor. From 1921-1952 he belonged to the Physical-Technical Institute in Leningrad.

Interruptions: 1918-1921 Krim-University Simferopol
1925-1926 Germany
1930-1931 USA
1941-1944 Kasan

He died on 23.1.1952 in Leningrad.

Frenkel was a universal theoretical physicist who was also open to experimentation and technology. His focus was condensed matter – solids, crystals, metals, liquids. He was one of the pioneers of quantum theory of the solid and liquid states of matter. In 1924 he proposed a first quantum theory of electron conductivity in metals, in 1926 the introduction of holes in the crystal lattice as quasiparticles and description of 'Frenkel defects' in crystals. In 1931 he introduced the 'excitation quanta' and in 1936 gave them the name excitons, one of the first quasiparticles. In 1932 he proposed the name 'phonon' for the 1930 by I.E. Tamm introduced 'sonic quantum',⁷ a quantized elastic wave in crystals. In 1936 and 1939 he developed independently from N. Bohr and J.A. Wheeler the droplet model of the atomic nucleus and an explanation of nuclear fission based on it.

He was highly recognized nationally and internationally. In 1929, he was elected a corresponding member of the Academy of Sciences of the Soviet Union.

During the Stalin era he narrowly survived campaigns against 'modern physics'.⁸ He had to justify himself for many years before state and party committees. In particular, he was pressed to 'take back' the books on Wave Mechanics⁹⁻¹¹ which he did naturally, if at all, only very half-heartedly and ambiguously.

FRENKEL published more than 250 articles and more than 30 books, often in many editions. Books translated into German or English are⁹⁻¹⁵ and secondary literature.⁸ The biography was written by the historian of science Viktor Ya. Frenkel, his son.

After the 2nd world war, the development with the FK model goes on in Germany by the work of Kochendörfer and Seeger,¹⁶ and in England by Frank and van der Merve,^{17,18} as well as by many other authors.¹⁹ Frenkel himself did not return to this model.

2.1 Introduction of the FK Model

The FK model describes a chain of particles, commonly atoms or molecules, see Fig. 1, which

1. are connected with each other by spring forces, and which
2. are attracted by another force, whose potential is described by a cosine function.

The springs are assumed to be equal, and the attraction into the base potential can be realized in many models: gravity, as in the pendulum model, or electrostatic or magnetic force.

The parameters of the model are:

- The initial distances of the atoms are a_0 .
- The 'spring constant' is k .
- The period of the cosine is a_s .

Mechanical pendulums, which are still coupled to each other by springs, form a special FK model, since the pendulums are fixed to their line.²⁰ The general model is displaceable above the base potential.

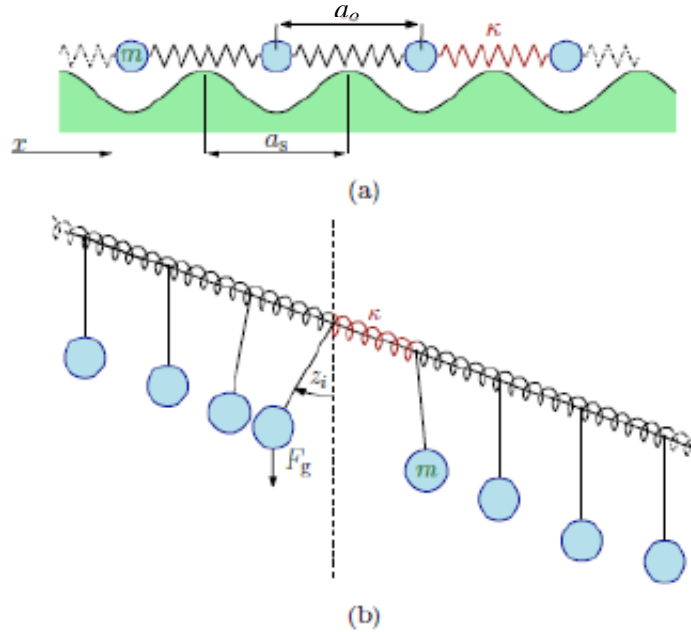


Figure 1: Frenkel-Kontorova Model (after Loi Do et al.²¹)

The potential for the linear FK chain of atoms $\mathbf{x} = (x_1, \dots, x_N)^T$ with $x_i < x_{i+1}$ is

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

The first sum describes the ground potential; each x_i sits anywhere in some cosine well. The combination with ‘1-cos’ is used to avoid negative values. The second sum describes the simplest form of a nearest neighbor relation with a harmonic spring approach. Both a shortening of the distance ($x_{i+1} - x_i$) below a_o , and an extension of this distance beyond a_o cause a force.

The boundary points x_1 and x_N are free (in the considered model).

Many generalizations have already been discussed: Other functions for the base potential,^{22,23} additively higher powers in the spring formula,^{24,25} or, in addition to the previous nearest-neighbor formula, the inclusion of additional neighbor atoms,^{26,27} which satisfy some weak versions of ferromagnetism, or using Coulomb forces.²⁸

In addition to free boundary values of linearly arranged FK chains, it is also possible to have cyclic FK chains that enforce periodic boundary values.²⁹

2.2 Two variants for the periods of the two potentials

- case of distances of atoms $a_o = a_s$ (same period).

The energy for the minimum of the FK chain is zero, because all particles can be at rest in the ground potential, and all spring forces are also at zero, see Fig. 2.

- Case of different distances of atoms $a_o \neq a_s$ (unequal period).

If the periods do not match, then the energy for the global minimum of the FK chain will be larger than zero, because not all particles can be in zero of the ground potential. Also possible spring forces are strained, see Fig. 3.

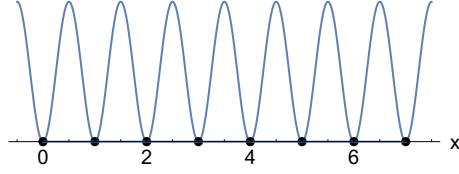


Figure 2: FK model with $N=8$ and $a_o = a_s$

In Fig. 3, there 8 atoms are sorted into 10 potential wells. This ground state has an energy larger than zero. (Some atoms are artificially drawn on the potential walls if they do not sit in zero energy wells.)

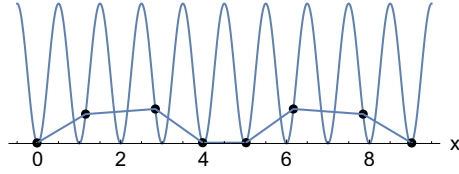


Figure 3: Minimum of the FK model, $N=8$, $a_o = 1.25 a_s$ and $k = 10V_o$

2.3 Global Minima, Saddle Points and Intermediate Minima

We move to a shorter 5-atom chain. For $a_o = 2/3 a_s$ this does not fit into the sinks of the ground potential. This results in the stationary points, global minimum (Min), saddle point (SP) of index 1 (SP_1) and intermediate minimum (int Min), shown in Fig. 4. The calculation uses common mathematical optimization methods.³⁰ Note that one already has a 5-dimensional problem at hand.

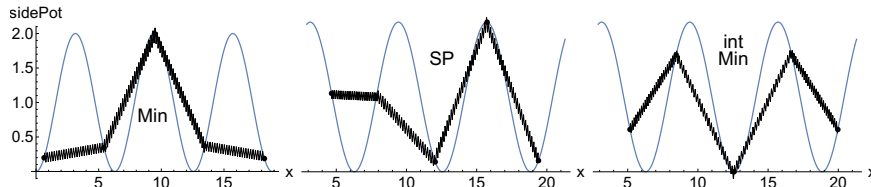


Figure 4: Stationary points of the FK model, $N=5$, $a_o = 2/3 a_s$, $a_s = 2\pi$, $k = V_o$

In the global minimum on the left hand side in Fig. 4 there are 5 atoms embedded in 4 sinks. In the minimum structure, one atom sits on the top of the ground potential. Any change in the chain leads to a higher energy. The Min structure can be shifted to the right so that one comes out at an SP_1 . A calculation for this is described below. The SP_1 has a much higher energy than the global minimum, but its neighboring intermediate minimum has almost the same energy. If one shifts the chain even further to the right (not shown), one can arrive again at a SP of index 1. This is mirror-symmetric to the SP of Fig. 4. A further rightward shift leads to a next global minimum, analogous to the left picture in Fig. 4, but a potential trough of the base potential further.

Fig. 5 shows an energy profile on the 5-dimensional potential energy surface (PES) from the global minimum, over SP_1 and Int-Min and a symmetric SP_1 to the next global minimum. It is an upper way in a high-altitude, nearly flat ‘mountain’ path for the FK model with $N=5$, $a_o = 2/3 a_s$ and $k = V_o$. A curve in the coordinate space of the FK chain was determined for this purpose (a Newton trajectory, see below), which connects the corresponding stationary points, and the energy above

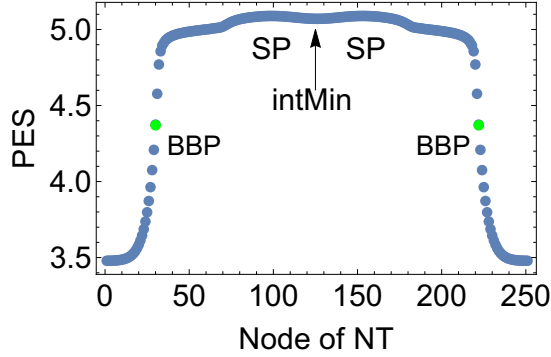


Figure 5: Energy profil for Fig. 4

the way is plotted from the potential of formula (1). The (green) points 'BBP' are also explained below.

3 Solitons

The observation of an almost flat 'mountain path' leads to the appearance of solitons in the case of longer chains. Solitons are structures which move through the ground potential similar to a particle, compare Fig. 6 and 7. Once formed, they need almost no further energy, but are very stable. The length L of the soliton extends over several troughs and peaks of the ground potential, but it is independent on the total length of the chain. It depends only on the parameters of the FK chain, i.e., on the periods of the potentials and on the sizes of the peaks, thus on the magnitudes V_0 and k , the scaling of the potentials. During a 'wandering' of the structure through the chain, at the front always new atoms are lifted, later moved over the next potential hill of the ground potential, and still later deposited in a more distant potential well of the ground potential. The structure of the soliton, however, remains the same. The term 'soliton' was proposed by Peyrard and Kruskal.³¹ It later gave the name to an entire field of research.

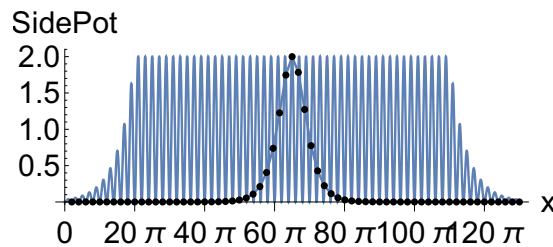


Figure 6: A soliton travels through the potential of a long chain.²⁸

3.1 Instantaneous images of a soliton

In Fig. 7 we have used a 10-atom chain with $a_o = a_s$. A push has been applied from the left, leading to the first SP_1 on the left, the first image on the upper left side. This requires a considerable amount of energy to be applied. After that, the structure can relax to an intermediate minimum to the right. Note that in particular the intermediate minima are stationary, i.e. stable states of the FK chain. However, once the first SP_1 is reached, a soliton, the compressed structure, can move

through the 10-atom chain until it reaches at the end the valley of the base potential, to which it further can relax again. A small energy barrier between the saddle points and the intermediate minima is still present. It is called the **Peierls-Nabarro** potential.³¹

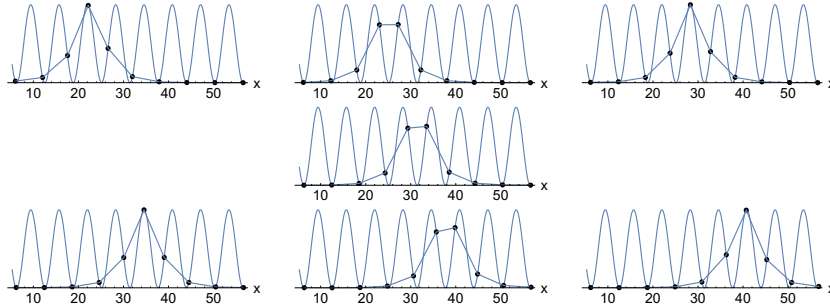


Figure 7: A soliton travels through the potential of a 10-atom chain with $a_0 = a_s$.

3.2 Soliton formula

Frenkel and Kontorova recognized in 1938 that the model contains the possibility of solitons. They assumed that there was already a dislocation (this was the name of a soliton at that time). For $a_o = a_s = a$ the displacement q_n of the n -th atom x_n is

$$q_n(t) = \frac{2a}{\pi} \arctan \left[e^{\pm \frac{2\pi}{L} (\pm vt - na)} \right].$$

L = length of the dislocation (of the soliton),

v = speed at which it travels, and

\pm shows the direction: dislocation moves to the right or left.

With $a = 1$, $L = 5$, $v = 1$, $n = 1$ the picture is given for the behavior of the first atom in Fig. 8.

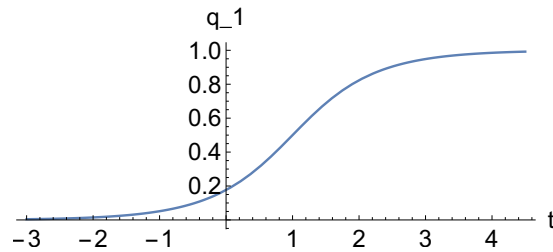


Figure 8: Graph of a soliton in atom 1.

q_1 of x_1 wanders from its potential well from its minimum x_1 with $q_1 = 0$ to the next at the distance $a = 1$, i.e. at the point $x_1 + 1$ with $q_1 = 1$. Thereby it overcomes the maximum of the fundamental potential in the 'center' of the drawn curve branch, above the number 1 of the first atom. These energy relations are not recognizable in the description of its path, but they can be traced in Fig. 7. For further atoms x_i with $i > 1$ the curve is shifted accordingly.

3.3 First Conclusion

- Without having considered dynamical equations, we can consider the steady states of the FK potential and develop the notion of a soliton.^{32–34}
- After a given excitation into a high intermediate state the FK chain forms solitons, which can also be imagined to migrate. However, the motion is slowed down by the Peierls-Nabarro barrier.

4 Excitations

We imagine another force vector $\mathbf{f}=F(f_1, \dots, f_N)^T$ of length F , where the N components f_1, \dots, f_N are fixed. The force acts per component on one atom of the chain. The simplest form for such a force is a linear approach with the scalar product of force vector \mathbf{f} and vector \mathbf{x} of the chain. This gives a new 'effective' potential

$$U_{eff}(\mathbf{x}) = U(\mathbf{x}) - \mathbf{f}^T \mathbf{x} \quad (2)$$

with the original FK potential $U(\mathbf{x})$. Its minimum is given by

$$\mathbf{0} = \nabla_{\mathbf{x}} U_{eff}(\mathbf{x}) = grad U(\mathbf{x}) - \mathbf{f}. \quad (3)$$

Curves where the gradient always points in the direction of \mathbf{f} , with increasing strength F of the force, are called Newton trajectories (NT), compare the important introductory works.^{35,36} NT have been studied in Leipzig for 25 years. They have been proposed for theoretical chemistry both as a method for SP search, and as a model for chemical reaction pathways themselves. A special application is in mechano-chemistry, where chemical reactions are controlled by an external force.^{37,38} We also applied the NT to the FK model.³⁰ For each given, fixed direction (f_1, \dots, f_N) there is a Newton trajectory. The special property of these curves is that they connect stationary points of an index difference of 1,³⁹ i.e. for example, they connect minima of index 0 with saddle points of index 1.

Above in Fig. 5 we started in the global minimum of a 5-chain. A Newton trajectory has connected all 5 low lying stationary points. Shown is the profile above the NT on the Potential-Energy-Surface (PES). The effort of the force F grows from 0 in the minimum to a 'barrier breaking point' (BBP), a point at which on the effective potential U_{eff} the barrier disappears.⁴⁰ After that, the length of the force vector F falls back to zero at the SP. And after that, the same game continues on the path to the intermediate minimum. Off this shown path there are SP with higher index and higher energy. But these are generally not of physical interest.

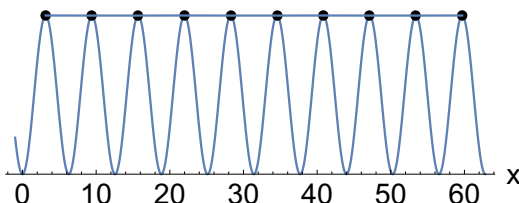


Figure 9: A maximal saddle point in a 10-atomic chain for $a_0 = a_s$.

With the existing theory of Newton trajectories we can follow how the excitations propagate through the FK chain, when a force vector is given and its strength is continuously changed.

An excitation that pushes all atoms simultaneously and uniformly such as $\mathbf{f}=F(1, 1, \dots, 1)^T$, is unfavorable from the amount because all atoms are pushed up their potential mountain at the same time, compare Fig. 9. A soliton structure, on the other hand, requires much less energy.

If the force is directed only to the left side of the chain and acts into the chain, like $\mathbf{f}=F(1, 0, \dots, 0)^T$, we will get a compressed structure, called antikink. On the contrary, a right-attacking force pulling out of the chain, $\mathbf{f}=F(0, \dots, 0, 1)^T$, will produce a stretched chain, called a kink, compare Fig. 10. On the left in Fig. 10 are 5 atoms distributed on 4 valleys, but on the right hand side, 5 atoms are stretched over 6 valleys.⁴¹ Both kink and antikink are solitons. For example, the stretched structure could move to the right as a soliton, or the compressed structure to the left, if the chain would be much longer than $N=10$. But if both structures move towards each other, then they cancel each other out.

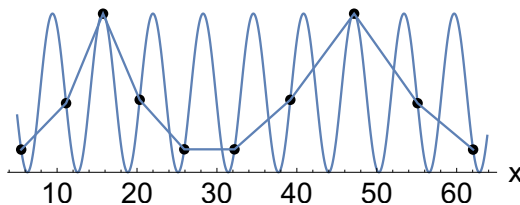


Figure 10: An antikink and a kink in a 10-atomic chain for $a_0 = a_s$.

5 Applications of the FK Model

5.1 Dislocations in crystals

The problem of dislocations in the lattice of crystals and their possible 'wanderings' was the starting point for this model. Kontorova and Frenkel had attempted to treat dislocations in 1938.²⁻⁶ This study was continued by Frank and van der Merve,^{17,18} and Kochendörfer and Seeger.¹⁶ The dynamics of vacancies in a polymeric crystal chain has been treated by E. A. Zubova.⁴²

5.2 Sliding processes between surfaces

Braun and Kivshar^{19,43} Chap. 5, treat in detail this application of the FK model. A kink slides on the base potential which is formed by the crystal surface or the nearest metal atoms. The substrate also serves for energy exchange. It plays the role of a thermostat.

Gangloff et al. also treat kinks for the study of nanofriction.^{44,45} They use additional forced motion for this purpose. Experimentally, they observe these processes at the atomic level.

Quapp and Bofill also propose the FK model for considering of sliding processes.^{41,46} Using NT, they calculate for a chain of medium length the saddle points for a sliding process.

5.3 Displacement of a Wigner crystal

In the work of the experimenters led by Jui Yin Lin^{47,48} a system of electrons was observed on a surface of supercold helium atoms. For this purpose, they had etched out a very narrow strip in which the helium atoms rested, and on it, so to speak, a one-dimensional chain of electrons is placed. These push in each case troughs into the surface, and they repel themselves with Coulomb

force. If one still fixes the edges of the chain, then one can treat with good will the chain of electrons as a Frenkel-Kontorova model.

In the experiment, the chain had been shifted by a force, and it had been observed, that one needs approximately the same force for chains of different lengths.

We proposed to understand this experiment by assuming the formation of a soliton.²⁸

5.4 Waves in fields of Josephson junctions

A Josephson junction is a quantum mechanical switching element which consists of two superconducting electrodes separated by an insulating barrier. The phase difference between the layers determines the behavior of these elements. Several such elements can be connected together to form chains, and even form a circle of them, in which the boundary values then become periodic. Ustinov considers phase differences in Josephson junction arrays as solitons.^{49,50}

Quapp and Bofill continue consideration of the FK model for Josephson junction arrays.⁵¹ Of particular interest are Shapiro jumps in arrays of Josephson junctions.⁵² They represent a dissipatively driven quantum effect. Larsen et al. observed the effect in graphene-based Josephson junctions.⁵³ Quapp and Bofill calculated Lyapunov exponents^{29,54} for the Langevin equation of the corresponding FK chain. They resulted in the bizarre situation of opposite Lyapunov exponents depending on the type of the boundary values of the FK chain.

5.5 Propagating Austenite-Martensite phase boundary

Austenite is the face-centered cubic modification (phase) of iron. The austenitic phase occurs between temperatures 1392°C and 911°C as γ iron. Martensite is a metastable microstructure in metals, alloys and also non-metals. It appears diffusionless and athermal by a cooperative shear movement from the parent initial microstructure.⁵⁵ In this process, the material must be heated from the temperature of a high-temperature phase (for steel: austenite) below the equilibrium temperature to a low-temperature phase (for steel: α phase, ferrite).

Alloys with shape memory are of particular interest here, such as nickel-titanium alloys. The latter materials exhibit these properties of interest already at ambient temperature.⁵⁶⁻⁵⁸ The supercooling below the equilibrium temperature must be deep enough to provide the necessary driving force for the athermal phase transformation.

For this purpose, Quapp and Bofill considered an FK problem generalized with respect to the base potential. The phase boundary was reduced to one layer, and a kind of soliton for the phase transition was calculated.²³ A Langevin solution was used to simulate this transition under a small external force.

5.6 Waves in DNA molecules and proteins

If regions of the inner bridges in the DNA molecule open up on a short piece of the strand, this structure can travel through the molecule like a wave.^{59,60} The process can be attempted to be described by an FK model.⁶¹

Also, the migration of loops in certain proteins, one can try to explain with an FK model.^{62,63}

6 Limit transitions

6.1 Limit transition to the continuum

We still want to investigate two limit processes for the FK model. On the one hand the transition from the discrete of the FK model to the continuous string, from the chain of oscillators to a vibrating string. This string moves according to the Sinus-Gordon equation, a well-known soliton equation^{50,64-66}

$$\frac{\partial^2 \phi}{\partial x^2} - \frac{\partial^2 \phi}{\partial t^2} = \sin \phi .$$

To the continuum limit: Let a chain consist of N atoms. In order to obtain the gradient for a dynamical consideration according to scheme 1 one has to derivate the energy formula after all N variables x_i .

The potential of the FK chain was given above

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

For a single particle x_i we have the potential contribution

$$V_o (1 - \cos(\frac{2\pi}{a_s} x_i)) + \frac{k}{2} (x_i - x_{i-1} - a_o)^2 + \frac{k}{2} (x_{i+1} - x_i - a_o)^2 .$$

Since each inner particle has a predecessor and a successor, it occurs twice in the part of the spring potential. We get as force acting on the i -th atom

$$\frac{\partial U(\mathbf{x})}{\partial x_i} = \tilde{V}_o \sin(\frac{2\pi}{a_s} x_i) - k(x_{i+1} + x_{i-1} - 2x_i) . \quad (4)$$

The first part of the formula is the derivative of the cosine summands, with $\tilde{V}_o = V_o 2\pi/a_s$, while the second part arises because there are always combinations of two atoms in the spring formula. We put the gradient into a Newtonian equation of motion of scheme 1. With Eq. (4) we obtain the discrete sine-Gordon equation, which is also used as a synonym for the FK model.²⁶

Now one can increase the number of atoms on a piece of the chain of fixed length and finally proceed to a continuum. The twofold difference part of the gradient of the potential in equation (4) then becomes a twofold derivative according to the spatial coordinate ϕ .

We treat the limit $N \rightarrow \infty$ and $x_i \rightarrow \phi(x)$, with $x_{i-1} \rightarrow \phi(x - a_o)$, $x_{i+1} \rightarrow \phi(x + a_o)$, and under $a_o \rightarrow 0$ one has to find the limit value for the 'spring constant' to be infinity $k := 1/a_o^2 \rightarrow \infty$.

It results with a twofold difference formula

$$k(x_{i+1} + x_{i-1} - 2x_i) = \frac{1}{a_o} \left(\frac{1}{a_o} (x_{i+1} - x_i) - \frac{1}{a_o} (x_i - x_{i-1}) \right) \rightarrow \frac{\partial^2 \phi}{\partial x^2} .$$

If one applies Newton's equation of motion

$$\frac{d^2 \phi}{dt^2} = -grad(U)$$

one obtains with the FK-potential the sine-Gordon equation

$$\frac{\partial^2 \phi}{\partial x^2} - \frac{\partial^2 \phi}{\partial t^2} = \sin \phi ,$$

the equation of a vibrating string. (The constant V_0 is omitted, and $a_s = 2\pi$ is set). Under the limit process also the former Peierls-Nabarro barrier disappears.

A one-soliton solution of this equation is again of the type, as was already found by Frenkel and Kontorova, the kink soliton (compare Fig. 11)

$$\phi = \phi(x,t) = 4 \arctan\left(\exp \frac{x - x_0 - vt}{\sqrt{1 - v^2}}\right), \quad |v| < 1 .$$

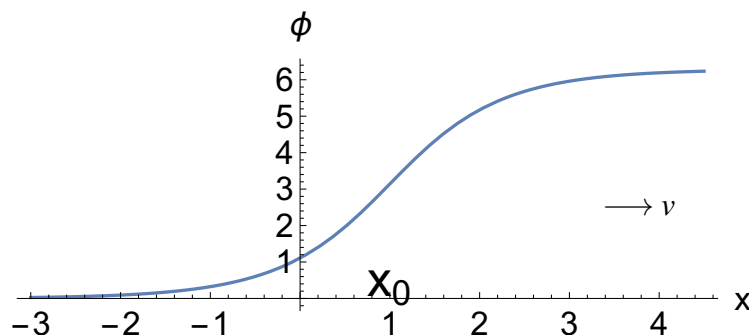


Figure 11: Wave soliton of the sine-Gordon equation with $x_0 = 1$.

$\phi(x,t)$ can be thought of as the angle of a pendulum fixed at x_0 . After the wave has passed through the point x_0 , the pendulum is rotated by 2π back to the same position. Frenkel and Kontorova arrived at this result using a different approach.

Another important equation in the central trio of soliton equations is the **Korteweg-de Vries equation**⁶⁷

$$\frac{\partial \phi}{\partial t} = 6 \frac{\partial \phi}{\partial x} + \frac{\partial^3 \phi}{\partial x^3} ,$$

a partial differential equation of third order. It describes solitons first observed in water channels by John Scott Russell in 1834.

As well as there is the **nonlinear Schrödinger equation**⁶⁸

$$i \frac{\partial \phi}{\partial t} + \frac{\partial^2 \phi}{\partial x^2} \pm |\phi|^2 \phi = 0 .$$

Both equations have been studied mathematically in many ways. Both allow soliton solutions in bell curve form.^{69,70}

7 Another limit

7.1 One extends the chain length to infinity

In the 1938 work on the FK model, Kontorova and Frenkel had used $a_o = a_s$, i.e., equal periods. Here above we have seen that a soliton is only short. In order not to have to deal with bound-

ary values of the chain, Kontorova and Frenkel had considered an infinitely long chain.² For the ground state of the FK chain, the energy at $a_o = a_s$ is zero, regardless of how long the chain is.

But in reality $a_o = a_s$ is rare.

We had seen above in Sect. 2.2 that for $a_o \neq a_s$ not all atoms can sit at the bottom of the potential well. Consequently, these deflected atoms have potential energy, and since also the springs between them are not always in zero deflection, energy must also be expended here.

This concerns with a hypothetically infinitely long chain consequently infinitely many atoms, so such a chain would have infinite energy, a physical impossibility.

Consequently, to consider infinite chains with different periodicity is not meaningful.

What was only a simplification of the consideration in the case of equal periodicity for Frenkel and Kontorova, now in the general case of different, not matching periodicities will become a nonsensical error for many users. So why one does consider infinite chains at all? We want to explain the reason.

We are looking for equilibrium states of the potential with equation (4), for gradient equal to zero. This gives a coupled system of equations

$$\frac{\partial U(\mathbf{x})}{\partial x_i} = \tilde{V}_o \sin\left(\frac{2\pi}{a_s} x_i\right) - k(x_{i+1} + x_{i-1} - 2x_i) = 0 \quad (5)$$

for all i in the chain, not for each of the two edge atoms. Thus, for atoms within the chain, the equilibrium formula does not contain the original distance a_o . However, this a_o remains in the two corresponding boundary equations for x_1, x_2 and x_{N-1}, x_N .

The system is a coupled one. One cannot simply evaluate individual equations without considering the others. This is a mathematical triviality which, however, must be remembered here.

7.2 The Fascination of the ‘Twist’ Transformation

If one sets for a pair of consecutive particles

$$P_i = (x_i, x_{i-1})$$

then one obtains for the $(N - 2)$ coupled equations ‘inside’ the chain a transformation, T , which repeats from equation to equation. With equation (5)

$$(x_{i+1}, x_i) = P_{i+1} = T P_i = (\tilde{V}_o \sin\left(\frac{2\pi}{a_s} x_i\right) - k(x_{i-1} - 2x_i), x_i) .$$

Since the sine function is periodic, one can still consider all values x_i modulo a_s and one obtains for $u_i = x_i \bmod(a_s)$ a 2-dimensional ‘twist’ transformation, which is repeated again and again.

One obtains, for example, a Fig. 12 of the results of a ‘twist map’.

Since this transformation is also area conserving, it has been used for a long time again and again to formulate statements about the FK model. But almost all statements about it unfortunately become wrong, if one considers a finite chain.⁷²

Where is the error in thinking?

The error is at the beginning of the chain. There is no way to know which equilibrium position will be reached for the two ‘first’ atoms, if one calculates a minimum. The supposed way out of many researchers was to move the ‘beginning’ to $-\infty$. But there nobody can start the calculation. So one somewhere starts and assumed that with this beginning an optimal structure will result later.

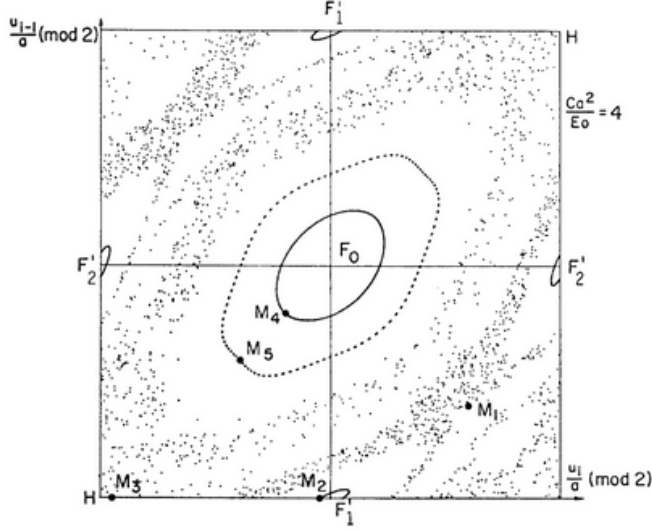


Figure 12: The points are repeated mappings with the twist map; the M_i are arbitrary starting points (after S. Aubry⁷¹)

An example of a flawed consideration is a 'theorem' by Baesens and MacKay,⁷³ in which the existence of limit cycles in a finite chain is asserted. This would imply that there is a relation of the type (for example, $3a_o = 2a_s$)

$$u_{i+3} = u_i + 2a_s .$$

However, for a chain of finite length, there always holds⁷²

$$u_{i+3} = u_i + 2a_s + \varepsilon_i$$

with a from particle to particle changing value of ε_i . At $N = 500$ we have found the smallest ε_i with $\varepsilon_{244} \approx 2 \times 10^{-11}$.⁷² The free edge values at the beginning and at the end of the chain destroy a fixed cycle.

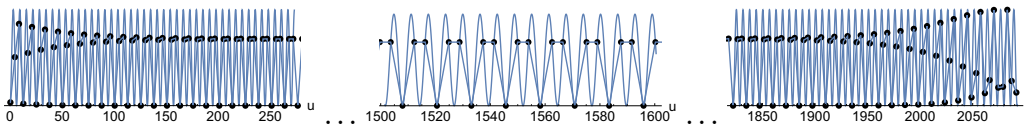


Figure 13: A left piece, a middle piece and a right piece of a chain with 500 atoms.

The center in Fig. 13 is an enlarged piece with the regular pattern representing the rational relation to a_s sorting three atoms in two wells. At the left edge of the chain, the influence of the free boundary values can be clearly seen. In the middle, a quasi-cycle has set in. Of course, the ε differences smaller than 10^{-2} cannot be resolved in the graphical representation. However, if a real limit cycle would result here, then at the right edge cannot again boundary values occur, which break out of the cycle.

We have recalculated this with the twist map. The structure of Fig. 13 was optimized, and with the so obtained 'correct' values x_1 and x_2 for a minimum structure, the twist map was started. Indeed, an analogous picture to Fig. 13 was obtained. Also the twist map finds the right 'output' at the correct start.

7.3 Outlook

We have been criticizing such false theories for years, but so far with moderate success.^{30,72,74,75} The draft of a corresponding commentary⁷⁵ was not accepted with a specious justification of *Phys. Rev. A*.

The sources for the twist map of the FK model have been quoted more than 1000 times; as far as we know only with small additions, never really negative. We have not yet been able to see that the authors in question now take our point of view.

According to Max Planck, new ideas do not prevail in research by convincing the followers of the old ideas. It is rather in such a way that the representatives of the old theory have to leave in order to make room for the new one.

Here, however, it is curiously reversed: It is enough to use the so to say ancient methods for the determination of stationary points to get along on the complicated potential-energy-surfaces of the FK model, supplemented possibly by the use of Newton trajectories. The ‘wrong’ detour via the twist map is not necessary.

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References

- (1) Quapp, W. *Das Frenkel-Kontorova Modell, Eine unendliche Geschichte*; Leibniz-Sozietät der Wissenschaften zu Berlin e.V.: www.math.uni-leipzig.de/MI/quapp/LS23FKmodelFebr.pdf, 2023; pp 1–40.
- (2) Kontorova, T. A.; Frenkel, Y. I. Zur Theorie der plastischen Deformationen und Versetzungen I (russisch). *Zh. Eksp. Teor. Fis.* **1938**, 8, 89–95.
- (3) Kontorova, T. A.; Frenkel, Y. I. Zur Theorie der plastischen Deformationen und Versetzungen II (russisch). *Zh. Eksp. Teor. Fis.* **1938**, 8, 1340–1348.
- (4) Kontorova, T. A.; Frenkel, Y. I. Zur Theorie der plastischen Deformationen und Versetzungen III (russisch). *Zh. Eksp. Teor. Fis.* **1938**, 8, 1349–1359.
- (5) Frenkel, Y. I.; Kontorova, T. A. To the theory of plastic deformations and twinnings. *Phys. Z. Sowjetunion* **1938**, 13, 1.
- (6) Frenkel, Y. I.; Kontorova, T. A. To the theory of plastic deformations and twinnings. *Fiz. Zh. (Moscow)* **1939**, 1, 137.
- (7) Vasileiadis, T.; Jeena Varghese, V. B.; Gomis-Bresco, J.; Urrios, D. N.; Graczykowski, B. Progress and perspectives on phononic crystals. *J. Appl. Phys.* **2021**, 129, 160901.
- (8) Frenkel, V. J. *Yakov Ilich Frenkel. His Work, Life and Letters*; Birkhäuser: Basel, 1996.

- (9) Frenkel, J. *Einführung in die Wellenmechanik*; Julius Springer: Berlin, 1929.
- (10) Frenkel, J. *Wave Mechanics: Elementary Theory*; Clarendon Press: Oxford, 1932.
- (11) Frenkel, J. *Wave Mechanics - Advanced General Theory*; Clarendon Press; Dover Publications, Inc: Oxford, 1934; 1950.
- (12) Frenkel, J. *Lehrbuch der Elektrodynamik I, II*; Julius Springer: Berlin, 1926,1928.
- (13) Frenkel, J. *Kinetic Theory of Liquids*; Clarendon Press: Oxford, 1946.
- (14) Frenkel, J. I. *Prinzipien der Theorie der Atomkerne*; Akademie Verlag: Berlin, 1957.
- (15) Frenkel, J. *Statistische Physik*; Akademie Verlag: Berlin, 1957.
- (16) Kochendörfer, A.; Seeger, A. Theorie der Versetzungen in eindimensionalen Atomreihen. I. Periodisch angeordnete Versetzungen. *Zeitschr. Phys.* **1950**, *127*, 533–550.
- (17) Frank, F. C.; van der Merwe, J. H. One-Dimensional Dislocations. I. Static Theory. *Proc. Royal Soc. London. Ser. A* **1949**, *198*, 205–216.
- (18) Frank, F. C.; van der Merwe, J. H. One-Dimensional Dislocations. II. Misfitting monolayers and oriented overgrowth. *Proc. Royal Soc. London. Ser. A* **1949**, *198*, 216–225.
- (19) Braun, O. M.; Kivshar, Y. S. The Frenkel-Kontorova Model, Concepts, Methods, and Applications. **2004**,
- (20) Basu Thakur, R.; English, L. Q.; Sievers, A. J. Driven intrinsic localized modes in a coupled pendulum array. *J. Phys. D: Appl. Phys.* **2008**, *41*, 015503.
- (21) Do, L.; Pucejdl, K.; Hurak, Z. Experimental Platform for Boundary Control of Mechanical Frenkel-Kontorova Model. *IEEE 61st Conference on Decision and Control (CDC)* **2022**, 7618–7623.
- (22) Milchev, A. Solitary waves in a Frenkel-Kontorova model with non-convex interactions. *Physica D* **1990**, *41*, 262–274.
- (23) Quapp, W.; Bofill, J. M. A generalized Frenkel-Kontorova model for a propagating Austenite-Martensite phase boundary - revisited numerically. *Eur. Phys. J. B* **2022**, *95*, 87.
- (24) Pelap, F. B.; Kamga, J. H.; Yamgoue, S. B.; Ngounou, S. M.; Ndecfo1, J. E. Dynamics and properties of waves in a modified Noguchi electrical transmission line. *Phys. Rev. E* **2015**, *91*, 022925.
- (25) Mounouna, F. G.; Wamba, E.; Nguetcho, A. S. T.; Bhat, I. A.; Bilbault, J. M. Modulational stability brought by cubic-quartic interactions of the nearest-neighbor in FK model subjected in a parametrized on-site potential. *Comm. Nonlin. Sci. Numer. Sim.* **2022**, *105*, 106008.
- (26) Mingaleev, S. F.; Gaididei, Y. B.; Majernikova, E.; Shpyrko, S. Kinks in the discrete sine-Gordon model with Kac-Baker long-range interactions. *Phys. Rev. E* **2000**, *61*, 4455–5561.
- (27) De La Llave, R.; Valdinoci, E. Ground states and critical points for generalized Frenkel-Kontorova models in \mathbf{Z}^d . *Nonlinearity* **2007**, *20*, 2409–2424.

- (28) 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.
- (29) 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.
- (30) Quapp, W.; Bofill, J. M. Newton Trajectories for the tilted Frenkel-Kontorova model. *Molec. Phys.* **2019**, *117*, 1541–1558.
- (31) Peyrard, M.; Kruskal, M. D. Kink dynamics in the highly discrete sine-Gordon system. *Physica D* **1984**, *14*, 88–102.
- (32) Guo, B.; Soliton Theory and Modern Physics, In *Soliton Theory and Its Applications*; Gu, C., Ed.; Springer, Zhejiang Sci., 1995; Chapter 1, pp 1–68.
- (33) Heyerhoff, M. *Die frühe Geschichte der Solitonen theorie, Dissertation*; Universität Greifswald, 1997.
- (34) Filippov, A. T. *The Versatile Soliton, Kap.6: Frenkel's Soliton*; Birkhäuser, Springer: Boston, 2010.
- (35) Quapp, W.; Hirsch, M.; Imig, O.; Heidrich, D. Searching for Saddle Points of Potential Energy Surfaces by Following a Reduced Gradient. *J. Comput. Chem.* **1998**, *19*, 1087–1100.
- (36) Quapp, W.; Hirsch, M.; Heidrich, D. Bifurcation of Reaction Pathways: the Set of Valley Ridge Inflection Points of a Simple Three-dimensional Potential Energy Surface. *Theor. Chem. Acc.* **1998**, *100*, 285–299.
- (37) Quapp, W.; Bofill, J. M.; Ribas-Ariño, J. Analysis of the Acting Forces in a Theory of Catalysis and Mechanochemistry. *J. Phys. Chem. A* **2017**, *121*, 2820–2838.
- (38) 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.
- (39) Hirsch, M.; Quapp, W. Reaction Channels of the Potential Energy Surface: Application of Newton Trajectories. *J. Molec. Struct., THEOCHEM* **2004**, *683*, 1–13.
- (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.
- (41) Quapp, W.; Bofill, J. M. Sliding Paths for Series of Frenkel-Kontorova Models - A Contribution to the Concept of 1D-superlubricity. *European Phys. J. B* **2019**, *92*, 193.
- (42) Zubova, E. A. On the Applicability of the Frenkel-Kontorova model to Describing the Dynamics of Vacancies in a Polymeric Crystal Chain. *J. Exp. Theoret. Phys.* **2001**, *93*, 895–902.
- (43) Braun, O. M.; Kivshar, Y. S. Nonlinear dynamics of the Frenkel-Kontorova model. *Phys. Rep.* **1998**, *306*, 1–108.
- (44) Gangloff, D.; Bylinskii, A.; Counts, I.; Jhe, W.; Vuletić, V. Velocity tuning of friction with two trapped atoms. *Nat. Phys.* **2015**, *11*, 915 – 919.

- (45) Gangloff, D. A.; Bylinskii, A.; Vuletić, V. Kinks and Nanofriction: Structural Phases in Few-Atom Chains. *Phys. Rev. Res.* **2020**, *2*, 013380.
- (46) Quapp, W.; Bofill, J. M. A Model for a Driven Frenkel-Kontorova Chain. *European Phys. J. B* **2019**, *92*, 95–117.
- (47) Lin, J.-Y.; Smorodin, A. V.; Badrutdinov, A. O.; Konstantinov, D. Sliding of an electron crystal of finite size on the surface of superfluid ^4He confined in a microchannel. *Phys. Rev. B* **2018**, *98*, 085412.
- (48) 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.
- (49) Ustinov, A. V. Solitons in Josephson-junction arrays. *Physica D* **1998**, *123*, 315–329.
- (50) Mazo, J. J.; Ustinov, A. V. In *The sine-Gordon Model and its Applications, Nonlinear Systems and Complexity*; Cuevas-Maraver et al., J., Ed.; Springer International Publishing Switzerland, 2014; Chapter 10, pp 155–175.
- (51) 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.
- (52) Shapiro, S. Josephson currents in superconducting tunneling: The effect of microwaves and other observations. *Phys. Rev. Lett.* **1963**, *11*, 80.
- (53) Larson, T. F. Q.; Zhao, L.; Arnault, E. G.; Wei, M.-T.; Seredinski, A.; Li, H.; Watanabe, K.; Taniguchi, T.; Amet, F.; Finkelstein, G. Zero Crossing Steps and Anomalous Shapiro Maps in Graphene Josephson Junctions. *Nano Lett.* **2020**, *20*, 6998–7003.
- (54) 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.
- (55) Otsuka, K.; Saxena, A.; Deng, J.; Ren, X. Mechanism of the shape memory effect in martensitic alloys: an assessment. *Phil. Mag.* **2011**, *91*, 4514–4535.
- (56) Xing, H.; Khantachawana, A.; Kim, H. Y.; Miyazaki, S. Effect of Ni-Content on Shape Memory Behavior of Ti-rich Ti-Ni Melt-spun Ribbons. *Mat. Sci. Forum* **2005**, *475-479*, 1925–1928.
- (57) Ko, W.-S.; Maisel, S. B.; Grabowski, B.; Jeon, J. B.; Neugebauer, J. Atomic scale processes of phase transformations in nanocrystalline NiTi shape-memory alloys. *Acta Materialia* **2017**, *123*, 90–101.
- (58) Plummer, G.; Mendeleev, M. I.; Lawson, J. W. Molecular dynamics simulations of austenite-martensite interface migration in NiTi alloy. *Phys. Rev. Mat.* **2022**, *6*, 123601.
- (59) Englander, S. W.; Kallenbach, N. R.; Heeger, A. J.; Krumhansl, J. A.; Litwint, S. Nature of the open state in long polynucleotide double helices: Possibility of soliton excitations. *Proc. Natl. Acad. Sci. USA* **1980**, *77*, 7222–7226.

- (60) Yomosa, S. Soliton excitations in deoxyribonucleic acid (DNA) double helices. *Phys. Rev. A* **1983**, *27*, 2120–2125.
- (61) Kulic, I. M.; Schiessel, H. Chromatin dynamics: Nucleosomes go mobile through twist defects. *Phys. Rev. Lett.* **2003**, *91*, 148103.
- (62) Sieradzan, A. K.; Niemi, A.; Peng, X. Peierls-Nabarro Barrier and Protein Loop Propagation. *Phys. Rev. E* **2014**, *90*, 062717.
- (63) Clopes, J.; Shin, J.; Jahnel, M.; Grill, S. W.; Ziburdaev, V. Thermal fluctuations assist mechanical signal propagation in coiled-coil proteins. *Phys. Rev. E* **2021**, *104*, 054403.
- (64) Barone, A.; Esposito, F.; Magee, C.; Scott, A. Theory and applications of the sine-Gordon equation. *Riv. Nuo. Cim.* **1971**, *1*, 227–267.
- (65) Scott, A. C.; Chu, F. Y. F.; McLaughlin, D. W. The Soliton: A New Concept in Applied Science. *Proc. IEEE* **1973**, *61*, 1443–1483.
- (66) Malomed, B. A. Soliton models: Traditional and novel, one- and multidimensional. *Low. Temp. Phys.* **2022**, *48*, 856.
- (67) He, B.; Meng, Q. Three kinds of periodic wave solutions and their limit forms for a modified KdV-type equation. *Nonlin. Dyn.* **2016**, *86*, 811–822.
- (68) Pelap, F. B.; Tatsinkou, I.; Fomethé, A. Nonlinear excitations in a continuous bi-inductance electrical line. *Phys. Scr.* **2011**, *83*, 045009.
- (69) N. J. Zabusky, M. D. K. Interaction of solitons in a collisionless plasma and the recurrence of initial states. *Phys. Rev. Lett.* **1965**, *15*, 240.
- (70) Zakharov, V. E.; Shabat, A. B. Exakte Theorie der zweidimensionalen Selbstfokussierung und eindimensionalen Selbstmodulation von Wellen in nichtlinearen Medien. *J. Exp. Theoret. Phys.* **1972**, *34*, 62.
- (71) Aubry, S. In *Solitons and Condensed Matter Physics*; Bishop, A. R., Schneider, T., Eds.; Solid State Sciences 8; Springer: Berlin, 1978; p 264.
- (72) Quapp, W.; Bofill, J. M. An analysis of some properties and of the use of the twist map for the finite Frenkel-Kontorova model. *Electronics* **2022**, *11*, 3295.
- (73) Baesens, C.; MacKay, R. S. Gradient dynamics of tilted Frenkel-Kontorova models. *Nonlinearity* **1998**, *11*, 949–964.
- (74) Quapp, W.; Bofill, J. M. Comment on ‘Out-of-equilibrium Frenkel-Kontorova model’ (A. Imperato, 2021, J. Stat. Mech. 013214). *J. Stat. Mech.* **2022**, 013204.
- (75) Quapp, W.; Bofill, J. M. Comment on realizing the Frenkel-Kontorova model with Rydberg-dressed atoms, by J.M. Muñoz et al, Phys. Rev. A 102, 043308 (2020). *Phys. Rev. A* **2022**, *rejected*, veröffentlicht als arXiv2210.070000, 1–5.