A model for a driven Frenkel–Kontorova chain

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Abstract. We study a Frenkel–Kontorova (FK) model of a finite chain with free-end boundary conditions. The model has two competing potentials. Newton trajectories are an ideal tool to understand the circumstances under a driving of an FK chain by external forces. To reach the insights we calculate some stationary structures for a chain with 23 particles. We search the lowest energy saddle points for a complete minimum energy path of the chain for a movement over the full period of the on-site potential, a sliding. If an additional tilting is set, then one is interested in barrier breakdown points (BBPs) on the potential energy surface for a critical tilting force named the static frictional force. In symmetric cases, such BBPs are often valley-ridge inflection points of the potential energy surface. We explain the theory and demonstrate it with an example. We propose a model for a DC drive, as well as an AC drive, of the chain using special directional vectors of the external force.

1 Introduction

In solid-state physics, one often divides a set of particles in a one-dimensional subsystem of interacting elements, and in the remaining part as a substrate. The latter acts by a potential on the extracted subsystem. One example of such a model is the Frenkel–Kontorova (FK) model [1,2]. It has the ability to account for many nonlinear problems. The one-dimensional subsystem is represented by a discrete chain of particles harmonically coupled with their nearest neighbors, while the action of the fixed substrate can be described by a sinusoidal form.

In many applications, one particularly interesting aspect of the FK model is its driven form. The concept has subsequently been involved in many applications of the model including alternating current (AC) driven models [2–6], or direct driven (DC) models [7–10]. Nowadays sliding friction forms a broad interdisciplinary research field that often involves the application of the FK model [8,10,11] where the applications go up to earthquake research [12]. Zanca et al. recently remarked that ‘friction is, among all basic physical phenomena, the one in most need of fundamental works’ [13].

We here propose the usage of Newton trajectories (NTs) [14]. They describe the curve of the displaced stationary points under the increasing external force for every tilted potential energy surface (PES). To treat the PES of a physical problem is not new; however it is here the key step for a deeper understanding. On the other hand, NTs are mathematical tools. They are curves on the given PES where at every curve point the gradient of the PES points into the same direction called the search direction [15]. With the help of NTs we find a low energy path (LEP) for a full movement of the chain through the PES over a period of the site-up potential. The search direction of the NT is the tilting direction of a force to be applied to move the chain exactly along this pathway.

The paper has the following sections: in Section 2 we report on the FK model which is then tilted in Section 3. A short review of the theory of NTs is added, and it is explained how NTs can be applied to the FK model. Section 5 describes an example of the N = 23 FK chain. We get symmetric and asymmetric minimums and saddle points (SPs) of indices 1 and 2. Here, the particularity emerges that the global lowest transition state on a minimum energy path (MEP) for a movement of the chain by \( \approx a_x \), the period of the sinusoidal potential, is a pair of two SPs of equal height in a row, with a valley-ridge inflection (VRI) manifold of points in between. Two such valleys emerge in the N = 23-case, separated by an SP of index 2. The connection of the two corresponding SPs is a family of singular NTs. Using these mathematical findings, we propose a model for an overall tilting of the chain along its axis by a special DC force, as well as by an AC force hopefully anticipating a corresponding experiment. The end is the Section 7. Data are collected in a Supplemental Material.
2 The FK model

2.1 Model formula

\( \mathbf{x} = (x_1, \ldots, x_N)^T \) is a linear chain of \( N \) discrete particles. The positions \( x_i \) are on an axis. For all particles holds \( x_i < x_{i+1} \). They are sorted in a fixed order. We treat a finite chain, thus \( N \) is less than infinity [14,16–23]. The boundaries are free [24].

A spring force acts with a force constant \( k \) between the particles which would results in a constant natural distance \( a_o \) of the particles. Without the side force, the end points of the chain are such that the average distance is \( a_o = (x_N - x_1)/(N-1) \). Different ‘natural’ distances are a possible generalization [25–28], as well as different spring constants, \( k_i \) [29], both of which we do not use here. A fixed on-site potential with a periodicity of \( a_s \) acts on the particles in concurrence with the springs. The sinusoidal potential mimics a rigid, not deformable substrate. The ratio \( a_o/a_s \) is named the misfit parameter. The PES for the variables \( x_i \) is the FK model

\[
V(\mathbf{x}) = v \sum_{i=1}^{N} \left[ 1 - \cos \left( \frac{2\pi x_i}{a_s} \right) \right] + \sum_{i=1}^{N-1} \frac{k}{2} \left[ x_{i+1} - x_i - a_o \right]^2. \tag{1}
\]

We put the factor at the sinusoidal potential, \( v = 1 \), throughout the paper. Then the spring constant, \( k \), is also the ratio of the strength of the sinusoidal potential to that of the spring potential. Because \( v > 0 \), the sinusoidal potential will modulate the chain [30], and we will generally get another average spacing, \( \tilde{a}_o \). All quantities referred to in this work are dimensionless.

2.2 Calculation of special structures of the FK chain

We use here the application of NTs as a method for the FK model [14]. For control reasons, we also use the optimization in Mathematica by ‘NMinimize’. A further tool is steepest descent (SD). Barrier breakdown points (BBPs) are calculated by the Barnes method [31]. VRIs are approximated by a scheme of Schmidt and Quapp [32,33].

3 Tilting of the FK model

In atomic force microscopy, a cantilever pulls a molecule with a given force in a defined direction [23,24]. Such a tilting can be applied also to an FK chain. Additionally to the two forces of the FK model, we use an external, linear force in the ansatz [1,2,14,19,26,34–43]. We name the resulting PES an effective PES

\[
V_F(\mathbf{x}) = V(\mathbf{x}) - F \cdot (l_1, \ldots, l_N)^T \cdot \mathbf{x}. \tag{2}
\]

The multiplication point between the normalized \( N \)-dimensional direction vector \( \mathbf{l} = (l_1, \ldots, l_N)^T \) and the \( N \)-variable \( x \) means the scalar product. The amount of the force is either given by the direct part, \( F_{dc} \) [7–10], or by an alternating part, \( \pm F_{ac} \) [2–5]. The force tilts the former sinusoidal potential with the incline \( F \) in direction \( \mathbf{l} \). If \( F = 0 \), then a minimum structure for the chain will exist. But if all \( l_i > 0 \), and if \( F > 0 \) is large enough, then a minimum does not exit [14,19]. Interesting is the so-called pinning–depinning transition, as well as the backward process [20], compare also Section 4.3 below. The barrier for a depinning is reduced in the case of special misfit parameters between chain and substrate. It was named superlubricity [44–49].

4 Newton trajectories

4.1 The definition

Tilting means that we now look for a stationary chain with \( g_i(\mathbf{x}) = F(l_i, i = 1, \ldots, N) \) is the variable amount and the \( l_i \) are fixed. Such an ansatz is named NT [50,51] in the \( N \)-dimensional space of the particles, to a search direction \( \mathbf{f} = F(l_1, \ldots, l_N)^T \). The stationary points on the effective potential satisfy the vector equation

\[
\nabla_x V_F(\mathbf{x}) = g(\mathbf{x}) - \mathbf{f} = 0. \tag{3}
\]

One searches a point where the gradient of the original PES, \( g(\mathbf{x}) \), has to be equal to the force, \( \mathbf{f} \). The NT describes a curve of force-displaced stationary points (FDSPs) of the tilted PES under a different load, \( F \) [50–56]. Usually, the energy of a minimum can increase, but the energy of the next SP can be lower. This means that the barriers become lower.

The NT can be treated without the treatment of the physics of the external force in equation (2). One only needs an abstract search direction. Then any NT describes a connection between different stationary points of an index difference of one [57]. Following an NT is a method to search a next SP if a minimum is given, or vice versa.

We write equation (3) in projector form [50,51]

\[
(U - 11^T) g(\mathbf{x}) = 0. \tag{4}
\]

\( U \) is the unit matrix and the \( 1 \)-unit vector is the normalized direction of \( \mathbf{f} \). The equation (4) then means that \( g \) and \( 1 \) are parallel. If we differentiate the projector equation (4) with respect to the parameter that characterizes the FDSPs curve, \( s \) in \( \mathbf{x}(s) \), we obtain with the Hessian, \( \mathbf{H} \) [51,53]

\[
(U - 11^T) \mathbf{H}(\mathbf{x}) \frac{dx}{ds} = 0. \tag{5}
\]

This is an expression of the tangent of the FDSPs curve. For the calculation, the continuous NT is approximated by \( L \) node points. The \( N \) particles of the chain form a point in the \( N \)-dimensional configuration space. A curve of such points is the NT. And it is numerically treated by its \( L \) nodes. We can easily calculate the Hessian of the FK model [14]. Then equation (5) is a way to generate the NT of a successive tilting. We use a predictor–corrector method for the calculations. For the predictor we use the tangent of the NT with equation (5), or the growing string ansatz [58,59]. The tangent of equation (5) is also
employed for the corrector direction, back to the correct NT, with a Newton–Raphsen-like method [59].

Note, the amount of the tilting force, \( F \), does not appear in equation \( (5) \). Thus, the NT of the original PES for \( F = 0 \) does not change if we jump to a special effective surface, \( V_F \), for a fixed \( l \)-direction and an \( F > 0 \).

### 4.2 Application of NTs to the FK model

We search for a minimum on the PES of the FK chain with the three steps:

1. Build a natural chain with spacing \( a_0 \); set, for example, \( x_1 = 0 \) for the initial particle, thus it is in the first well of the sinusoidal potential, and set \( x_i = (i - 1) a_0 \) for \( i = 2, \ldots, N \).
2. Use the natural chain in the PES of equation \( (1) \); it gives \( V(x) \), and calculate the gradient \( g(x) \).
3. Form the normalized direction \( l \) along the negative gradient: it is the search direction of an NT which goes through the surface point \( V(x) \). Follow the NT downhill to the next stationary state which usually is a minimum.
4. By turning the search direction starting at a minimum, we find SPs in the same way because NTs equivalently work downhill or uphill. This property is connected with the index theorem [57] which determines that regular NTs connect stationary points of an index difference of one.

### 4.3 Barrier breakdown points – BBPs

If one goes along the corresponding FDSPs curve with a given direction \( l \), then the magnitude of the gradient, equal to \( F \), is zero at a stationary point of \( V(x) \), and ends with zero at the final next stationary point. In between there has to be a maximum of \( |g| \). Here holds the condition [55,60,61].

\[
\text{Det}(H(x)) = 0 \quad (6)
\]

with the Hessian, \( H(x) \), of the original PES, \( V(x) \). This is the point where the effective \( V_F(x) \) along the FDSPs path has a shoulder [55,60,61]. The barrier of \( V_F(x) \) decreases from the original PES barrier to zero. The point on the FDSPs curve is named the BBP. Then the critical force, \( F_c \), named the static frictional force [8], is so high that it causes the final depinning of the chain.

If we compare all NTs of a set which connect the same minimum and SP, then the NT which gives the lowest value of \( F_c \) is the optimal NT, and the point is named the optimal BBP [55,61]. The optimal BBP defines the lowest maximal magnitude of the force. It satisfies the equation [55,61]

\[
H(x)g(x) = 0 \quad \text{where} \quad g(x) \neq 0. \quad (7)
\]

At the optimal BBP the gradient is an eigenvector of the Hessian matrix to eigenvalue zero. The point belongs to a gradient extremal (GE) [62–68]. At the optimal BBP, the \( \text{Det}(H) = 0 \)-manifold, the GE and the optimal regular NT meet. An algorithm to locate optimal BBPs has recently been proposed [31]. The expression of the optimal BBP, equation \( (7) \), has a special form for the FK-model because of the tridiagonal shape of the Hessian, see reference [14].

### 4.4 Degenerated stationary points

On the PES of the FK model for \( N=23 \) particles many degenerated stationary points emerge. They are defined by the condition

\[
|g(x)| + |\text{Det}(H(x))| = 0. \quad (8)
\]

For NTs such points are quasi ‘regular’ points where the index theorem [57] does not apply. We demonstrate it by a simple 2D example in Figure 1. (There are equidistant contours drawn by Mathematica, version 11.2, like all other figures of this paper). We study the behavior of NTs near a shoulder on a ridge where condition \( (8) \) is fulfilled.

The index theorem does not say what happens, because the shoulder is a stationary point of a ‘half’ index: the gradient is the zero vector, but also an eigenvalue of the Hessian is zero. The shoulder point behaves like an ordinary point of the PES. The green lines are BBPs of NTs.

### 5 Example of the FK chain with 23 particles

Experiments with a chain of few tens of ions are done [24,69]. The chain we will be looking at is the case \( N = 23 \), with the parameters \( a_s = 2\pi, a_0 = 4\pi/3, v = k = 1 \) (thus the misfit parameter is 2/3).
For Figure 2 we move the rigid natural chain with fixed equal distances, $a_0$, between all atoms, by $2\pi$ over the on-site potential and draw the energy profile. Because the on-site potential is fixed, we get different energies for the chain. We do not use an NT for the movement of the fixed chain, but the direction of the movement itself is the standard one, $(1,\ldots,1)^T$. The minimum emerges at $a_0$ and the maximum at $24$. The energy difference of the profile of Figure 2 exhausts with 2 units the value of the $(1 - \cos(x))$ function of the FK model [18]. Note that for the natural chain the part of the spring energy is zero. At the mean energy, 23, the 23 cosine terms of the chain part of the spring energy is zero. At the mean function of the FK model [18]. Note that for the natural first step up to the SP the atoms $x_1$ are distributed to 16 wells of the sinusoidal potential. The occupation numbers 1 and 2 alternate here. For the minimum is $\tilde{\alpha}_0$; for the full 23-dimensional PES of the chain we localize the corresponding stationary points. The left two are the zero well of the site potential like in Fig. 3), and with a complementary minimum on the other side of the PES mountains moved by $a_0 = 2\pi$ over the sinusoidal potential. This is the aim: we search for a recurrence of the initial state of the chain moved over the site-up potential. The SP$_2$ has two equal negative eigenvalues of $-0.3813$. To give an image of the region around this top we draw a 2D sectional picture of the PES of the FK model (1) for $N = 23$. We used the two negative eigenvectors of the SP$_2$ for the plane of the picture; the data are in the SM, Section 2.1. The points of the plane are obtained by the linear ansatz $x(s, a) = SP_2 + s EV_1 + a EV_2$ and are included in the energy function, $V(x)$. The result is Figure 5. It is a representation of the simplified energy function $V_{SP_2}(x(s, a))$ by level lines. Note that it is a 2D section. The point $(0,0)$ is exactly the SP$_2$; however, stationary points lying displaced may not be correctly represented. Since 30 years, SPs of index 2 are discussed in theoretical chemistry [70–77]. Here emerges a possible Characterization of an SP$_2$:

- From a usual SP of index 1 one can expect to go down by the SD into two different minimum valleys using for the first step the eigenvector to the negative eigenvalue.
- From an SP of index 2 one can hope that it is possible to go down by the SD into up to four different minima using for the first step the two eigenvectors to negative eigenvalues. (But many other cases are possible; one is studied in references [78,79]).

We have four SPs of index one on a circle around the SP$_2$. On the full 23-dimensional PES of the chain we localized the corresponding stationary points. The left two are on the level 21.1699, the right two at the slightly higher energy 21.2106 (in contrast to the relation in Fig. 5). The data are in the SM in Section 2.2. An equipotential line

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**Fig. 2.** Energy profile of the equidistant 23 particles (the natural chain) moved over the on-site potential as a fixed chain by a total distance of $2\pi$. The horizontal axis depicts the location of $x_1$. The curve is a hint that for “useful” connected structures, from one stationary point to the next at $2\pi$ distance, the energy should not exceed this 24 units mark.
Fig. 3. Schematic picture of the structures of the ‘left’ asymmetric global minimum of the 23-particles chain, and its mirror image, the ‘right’ asymmetric minimum. The energy is 19.8242. Note that the particles are artificially set to the value of the \((1-\cos)\)-function. The real chain is linearly ordered on its axis. Only the distances between the \(x_i\) are changed by the on-site potential.

Fig. 4. An SP of index 2 of the 23-particle chain depicted by SP\(_2\) in the simplified Figure 5. The energy is 22.099. It is symmetric.

connects the two left SP\(_l\), as well as another equipotential line connects the two right SP\(_r\). The corresponding pieces are part of an NT to direction ‘sym’, here in this simplified 2D picture. It means that all gradients of the 2D sectional PES on this curve point into ‘sym’-direction. Note that the NT can pass a point where its tangent is orthogonal to the gradient: at the symmetric VRI points.

From ‘gMin’ at the bottom of Figure 5 to ‘2\(\pi+gMin\)’ at the top, we find two valleys through the PES, one may be the MEP over the two lower SPs of index 1, but the other is an LEP quite parallel to the former. Which valley we choose for a movement of the chain by a tilting force depends on the direction of the describing NT of the corresponding valley, see the description below.

The singular NT divides the two different valleys. It has a branch which forms the line \(\text{asym} = 0\) in Figure 5. The two red points on the line are the bifurcation points of the NT which are VRI points of the surface between the two intermediate minimums, iMin, and the SP\(_2\). Thus, the NT is a singular NT [51]. (Two other asymmetric VRI points are also included in the figure, near the \(\text{asym} = 0\) line at the green crosses. The corresponding singular NTs through the asymmetric VRI points are given in Figs. 6 and 7.) The symmetric VRI points on the line \(\text{asym} = 0\) are also BBPs because they are intersected by two green lines. But we cannot classify these BBPs to be ‘optimal’ because the NT is singular. Other NTs for a comparison do not connect the two SP\(_l\), or the two SP\(_r\), because of the index theorem [57]. On the line \(\text{asym} = 0\), of course, it holds at the BBPs that \(|g|\) is a maximum. Such a maximum fits well the NT theory at VRIs [55].

Fig. 5. A region of the PES is approximated around the global SP\(_2\) at (0,0). The axes are the two negative eigenvectors of the full Hessian at the SP\(_2\). They are symmetric or asymmetric directions. The thick curve is a singular NT to direction ‘sym’. The 4 red points are VRI points. The green bullets are BBPs of the singular NT, and the net of green lines indicates \(\text{Det}(H) = 0\). The description of the SPs of index 1 goes with ‘\(l\)’ for left, ‘\(r\)’ for right, ‘\(b\)’ for bottom, and ‘\(t\)’ for top, in this figure. gMin depicts the two (global) minimums of the (full) PES. In this 2D simplification of the PES the iMin\(_1\) is still deeper.

Figure 8 represents a regular NT through the two ‘right’ SP\(_1\). The structure of the SP\(_1^{\text{lb}}\) is shown in Figure 9, where the structure of the SP\(_1^{\text{rb}}\) is shown in Figure 10. The SPs at the top of the corresponding Figure 5 are mirror structures of the SPs below. The data are in the SM, Section 2.2. The NT of Figure 8 may be one of the interesting NTs which describes an LEP of the chain over a distance of \(2\pi\), the periodicity of the site potential. Below we will examine its use in the full 23D coordinate space.

Note that NTs are sometimes good models for reaction pathways over a PES. Here, they serve for paths
Fig. 6. The singular NT through the ‘lower’ asymmetric VRI point in the 2D simplified PES of Figure 5.

Fig. 7. The singular NT through the ‘upper’ asymmetric VRI point in the 2D simplified PES of Figure 5.

which describe the FDSPs curve. They connect different stationary points in an understandable and continuous way, and they can be used for a tilting of the chain into the corresponding direction.

Another method for the study of the PES is the SD from the upper stationary points. Thus, the global connection of the region around SP\(_2\) is easy to explore by the SD for the full 23-chain. We can start the SD curves at the SP\(_2\) in the direction of its negative eigenvectors, or at the corresponding SP\(_1\) in a diagonal direction. We have 4 valleys going downhill; two meet at the bottom and two at the top of Figure 5, which we always use for the illustration but leaving out the other hidden 21 dimensions of the full chain. Two other valleys meet at the intermediate iMin1, and two at the intermediate iMin2. Thus, SP\(_1^{lb}\) connects the global ‘right’ minimum with iMin2, SP\(_1^{rb}\) connects the global ‘left’ minimum+2\(\pi\) with iMin2, SP\(_1^{lt}\) connects the

Fig. 8. The regular NT to direction ‘asym’ connects the two global minimums over the two ‘right’ SP\(_1\) and the ‘right’ intermediate minimum, on the simplified 2D plane. Thus, it could be one of the NTs of interest for a global low energy path of the chain.

Fig. 9. The SP\(_1^{lb}\) of the 23-particle chain, compare Figure 5. The energy is 21.1699. It is asymmetric. Its mirror structure is SP\(_1^{lt}\).

Fig. 10. The SP\(_1^{rb}\) of the 23-particle chain, compare Figure 5. The energy is 21.2106. It is asymmetric. Its mirror structure is SP\(_1^{rt}\).
global ‘right’ minimum with iMin1, and SP$^r_1$ connects the global ‘left’ minimum +2π with iMin1. This means equivalently that the vertical direction of the NT leads to the global ‘right’ minimum below, and to the global ‘left’ minimum +2π at the top. Thus, a vertical pathway like one of the corresponding branches of the shown NT of Figure 8 will form a global LEP of the chain. The first peculiarity is that there are two competing ways, one on the left hand side, and one on the right hand side. The second peculiarity is that there are two SPs of index one in a row. An LEP on the tilted PES of the chain would have to pass both SPs on one side, one after the other.

For the full 23-chain, location and energy change for the numerical relations between the diverse stationary points; however, the ‘topological’ relations continue to stay like in Figure 5.

The horizontal direction along the asym = 0 line leads downhill from SP$^r_2$ to two intermediate minimums. This is also the result of an SD in the ±-symmetric direction from the SP$^r_2$. The structure of the minimums is shown in Figures 11 and 12; and the data are in the SM, in Section 3. The intermediate minimum, iMin2, is symmetric. It is a compressed structure, $\tilde{a}_0 = 3.98$. The ends of its structure are pushed into the center by $\approx 2\pi$. The intermediate minimum, iMin1, is also symmetric, but it is a stretched structure, $\tilde{a}_0 = 4.48$ (remember $a_0 = 4.19$). An imagination of a vibration between the two intermediates ‘flowing’ around the SP$^r_2$, more or less in the symmetric hyperspace of the chain, would be a ‘breathing’ of the chain, but not a translation of the chain by $2\pi$.

On the line asym = 0 the tilting moves together, or moves apart, the symmetric stationary points: the SP$^r_2$ and alternatively the two symmetric intermediate minimums.

For a moderate $F > 0$, say 0.2, it moves together the SP$^r_2$ and the right symmetric minimum. This means that the iMin1 is increased in energy, see Figure 13. Under this action, the two right SP$^r_1$ also move up in energy, so that the two left SP$^l_1$ become much lower, and the MEP clearly goes over the left iMin2. But the level lines between the left as well as the right SP$^l_1$ survive because the SPs move together on the singular NT which also survives.

For a moderate $F < 0$ the tilting moves together the SP$^r_2$ and the left symmetric minimum, vice versa to the former case, see Figure 14. At least, for a critical $F^c$, the 2D-summit of SP$^r_2$ and the corresponding former intermediate minimum coalesce, as well as the two SP$^l_1$, and only one path along the level line along the singular NT.
Fig. 14. Tilting the PES to the right hand side by a force into minus ‘sym’ direction.

Fig. 15. Tilting the PES to the top of the region by a force into ‘asym’ direction with \( F = 0.275 \). The light brown curves are two singular NTs through the asymmetric VRIs (see Figs. 6 and 7) which are the borders of the channel for a useful regular NT [56].

remains. A corresponding strong tilting makes the corresponding symmetric, former intermediate minimum to the global minimum, at least on the simple 2D section of Figure 5.

On the other hand, a tilting along the asymmetric eigenvector, in vertical direction in Figure 5, leads at least to a dramatic disappearance of one global and the left intermediate minimum, and of the SP2, and of three SP1, compare Figure 15. For \( F = 0.275 \) the global minimum at the bottom (with \( x_1 \) near 0 on the axis) and the right intermediate minimum 1 survive. For \( F = -0.275 \) the global minimum at the top (with \( x_1 \) near 2\( \pi \) on the axis) and again the right intermediate minimum 1 survive.

Now we leave the tool of the 2D approximation of Figure 5, even though we already had associated corresponding patterns of the approximation with real structures of the chain. For the 23-chain, we first show a connection between the two right SP1 by two different NTs in Figure 16. The search directions are the two SP directions. The combined curve opens a connection between the two global minimums, one at the initial location, but the second at a 2\( \pi \) moved structure. An external stimulation in the corresponding directions would need an AC-like force for a first step to move the chain into the iMin1, and a second step to move it to the ‘upper’ global minimum. However, it seems quite complicated to generate such forces because not only the ± changes are needed but also a change of the direction to its mirror direction in the 23D space.

In Figure 17 is shown the same calculation for the SPs of index one on the left hand side of the SP2.

5.3 Symmetric VRI points between iMin1 and SP2

To guess the search direction for singular NTs is possible [32,33]. In full 23 dimensions, we first test the NT to the ‘sym’ direction of the SP2: does it fulfill the task as it does in the simplified 2D case to be a singular NT? The proof is doing an NT calculation to the negative symmetric eigenvector direction of the SP2. The (more or less) positive result is given in Figure 18. It is an automatic detection of a VRI point to the sym-direction of the SP2.
Fig. 17. Energy profile over an MEP on the PES crossing the two SP\textsubscript{1} at 21.1699. The two left NTs are calculated to the SP-eigenvector at the bottom-SP\textsubscript{1}\textsubscript{lb}, where the two right NTs are calculated to the SP-eigenvector at the top-SP\textsubscript{1}\textsubscript{lt}. Start is in all cases the corresponding SP, and the four pieces are combined. At the iMin\textsubscript{2} two NTs again cross which belong to different directions. All stationary points are depicted by black bullets; further small peaks of the inner NTs are turning points (TPs).

Fig. 18. Energy profile over an NT to the symmetric EV-direction of the SP\textsubscript{2}. Start is the SP\textsubscript{rb} where the NT follows the direction up to the VRI point at 21.46. The NT follows the mirror branch after the VRI to the SP\textsubscript{rt}. This takes place by the NT to the given direction starting at the SP\textsubscript{tb}. The energy profile over the NT crosses the symmetry subspace of the chain at the corresponding VRI point at 21.46, see Figure 18. However, note that the level of this VRI point is quite higher than the level of the SP\textsubscript{r}. So, one can guess that the sym-direction of the SP\textsubscript{2} is not an optimal direction for an external stimulation of the chain.

The search of further symmetric VRIs is done by the variational program of Quapp and Schmidt [32,33]. The aim is to find a ‘better’ singular NT which connects the two right central SP\textsubscript{1} over this VRI point. The NT will be a tool to push and pull the FK chain globally over the PES by $2\pi$. Three further VRIs are detected by test calculations. We assume that between them a manifold of VRI points exists [57,80–83].

Remark: The chemical community ignores the fact, up to date, that usually not only a single VRI point exists, but also the VRIs are connected in a larger VRI-manifold. It is like in the case of conical intersections. Here, we have the same problem of the ‘unimaginability’ of higher dimensional connected points of such a character, see references [84,85] and further references therein.

The data of the VRI points are given in the SM, Section 3.3. The VRI1 is at energy 20.6710 with $|Ag|=1.459\text{E}-002$. ($A$ is the adjoint matrix to the Hessian, $H$. $|Ag|=0$ is the VRI criterion.) The NT to the corresponding direction of the gradient here, by the growing string method [58,59,78], is shown in Figure 19 together with other NTs. The curve in the symmetric subspace of iMin\textsubscript{1} and SP\textsubscript{2} is well calculated with convergent corrector steps. We use here the growing string method to really enforce the NT to finish at the SP\textsubscript{2}. It thus has to cross the VRI point on its way; but it does not break out to a side branch of the singular NT to one of the two SP\textsubscript{r}. (In the next subsection, we use the other kind of calculations following the tangent of the NTs.)

The VRI2 is at energy 20.92 with $|Ag|=3.843\text{E}-003$. The next corresponding NT is shown again in Figure 19. The VRI3 is at energy 21.0913 with $|Ag|=1.507\text{E}-003$. The level of this VRI point is nearest to the corresponding SP\textsubscript{r}-level. The structure of the VRI3 point is shown in Figure 20. The NT is shown in Figure 19. The NTs to the 3 lower VRIs show a TP. Nevertheless, they are fully in the symmetric subspace of the 23-chain. Note additionally that the curves are depicted over their nodes of the NT calculation. The distances in the coordinate space, from node to node, may not be equidistant because of the predictor-corrector scheme of the calculation.
Fig. 21. Energy profile over an NT to direction of the symmetric VRI3 point. Start is the iMin1 where the NT follows the direction to SP\textsubscript{2}\textsuperscript{rt} uphill up to the VRI point at 21.091. There it jumps to one of the crosswise branches from the VRI point to the SP\textsubscript{1}\textsuperscript{tt} of index 1. The NT crosses the SP and goes further downhill to the global minimum moved by 2\pi. Further seemingly peaks are TPs.

Fig. 22. Energy profile over an NT to direction of the symmetric VRI3 point. Start is the SP\textsubscript{1}\textsuperscript{rb} where the NT follows the direction to the VRI point at 21.091. It follows the mirror branch after the VRI to the SP\textsubscript{1}\textsuperscript{lt}. The branch between the VRI point and the SP\textsubscript{1}\textsuperscript{tt} is also a part of Figure 21.

5.4 Branches of the singular NT between the two SP\textsubscript{1} and the iMin\textsubscript{1}

The found 3 VRI points deliver the directions for 3 singular NTs which connect the two SP\textsubscript{1}, and which also have a branch to the intermediate iMin1. They are calculated with an NT following program using the tangent of the NTs with equation (5) for a predictor step. The results are shown in Figures 21–23. Now the calculation of the corresponding NTs can jump to a side branch of the singular NT at the VRI point, in Figures 21 and 23 as well. Interestingly, in Figure 22 the NT follows the tangent and jumps over the VRI point to the other side branch.

5.5 Singular NTs between the two SP\textsubscript{1} and the iMin\textsubscript{2}

We will again get an automatic detection of the VRI to the sym-direction of the SP\textsubscript{2} starting now at the left SP\textsubscript{1}\textsuperscript{lb}. The energy profile over the NT crosses the symmetry subspace of the chain at the corresponding VRI point at 21.687, see Figure 24. Note that the level of this VRI point is quite higher than the level of the SP\textsubscript{1}. So, one can guess that the sym-direction of the SP\textsubscript{2} is not again an optimal direction for a stimulation.

6 Calculations on the tilted PES

6.1 Symmetric force AC driving to new stationary states

We apply equation (2) with the direction vector being the gradient at a selected VRI point of the symmetric subspace of the chain, \((g_1,\ldots,g_N)^T\). The vector is also symmetric. For Figure 25 we use the gradient vector of the VRI3 as an example. To make the profiles for different amounts, \(F\), comparable, we represent relative energies. The global minimum (moved by 2\pi) at the end of the NTs (on the right hand side) is always put to zero. Near the factor \(F = -0.15\) the iMin1 and the former global minimum change the order; the intermediate minimum becomes the global one. A similar scheme of NTs exists for the other side of the iMin1 valley, for the connection from the global minimum (beginning with \(x_1\) in the zero-bowl of the site-potential) over SP\textsubscript{1}\textsuperscript{lb} to the iMin1. On the
Fig. 25. Tilting of the chain. Relative energy profiles over NTs to the symmetric gradient direction of the VRI3. One can imagine the profiles as MEPs on the effective PESs (where the peak at the VRI point can be omitted). Start is the iMin1 on the left hand side. The NT follows the valley to the VRI point, then turns to the SP\textsuperscript{rt} and goes downhill to the global minimum moved by 2\pi. All curves are fixed at zero at the former global minimum, for better comparison. From top to bottom we used the factors \(F = 0, -0.15, -0.2, \) and \(-0.35.\) The red curve for \(F = 0\) corresponds to the not tilted NT in Figures 21 and 22.

other side of the SP\textsubscript{2}, the iMin2 is increased in energy, for the used tilting, compare Figure 14.

With usual thermodynamics, one can assume that under such a force the chain jumps from a global minimum to the iMin1, if the system temperature is higher than the remaining SP. If the force is stopped, the chain can relax, and by the symmetry, it will jump back with a probability 1/2 to the global minimum, or to the global minimum moved by 2\pi. Thus, with probability 1/2 we would get a global movement of the chain for such an AC driven system. Interestingly, the driving direction along a symmetric VRI-gradient will be orthogonal to the global moving direction of such a process.

6.2 Asymmetric force DC driving to new stationary states

We use the first asymmetric eigenvector to the negative eigenvalue of the central SP\textsubscript{2}. The energy profile of a continuous NT starting at the global minimum to this direction is shown in Figure 26.

We again apply equation (2) with the direction vector being the negative asymmetric eigenvector of SP\textsubscript{2}. We use \(F = 0, -0.05, \) and \(-0.1\) in Figure 27. To make the profiles for the different amounts of \(F\) comparable, we show relative energies. The global minimum (moved by 2\pi) at the end of the NTs (on the right hand side) is always put to zero. With usual thermodynamics, one can assume that under such a force the chain crosses from the global minimum to the iMin1, if the system temperature is higher than the remaining SP. The way to the other global minimum moved by 2\pi is still easier then. The blue curve may describe the stationary points of such a DC driven system.

At the end of this subsection we remark that finding such an asymmetric driving direction, in a general high-dimensional PES, may be difficult. One has to detect the narrow pass, here for one dimension of the 23 dimensions of the chain, which meets the region of the central SP\textsubscript{2}. A 3D schematic picture of the former Figure 5 may illustrate this, see Figure 28.

6.3 Push and pull force DC driving to new stationary states

The asymmetric direction for a driving force in Section 6.2 may be quite complicated to realize for an experiment. But a main property of the direction is that the main components of the force are concentrated at the periphery. This is why we tried a simpler direction, \((1,0,\ldots,0,1)^T,\) like it was used also in the case \(N = 5\) in reference [14]. The NT to the direction is successful for a connection of the global minimum over the SP\textsubscript{1b} to iMin2 and over the
Fig. 28. 3D version of the 2D-schematic PES section of the 23-chain. The hill at the center is the central SP

SP

down to the 2π moved global minimum. Note: it is the other way around the SP
down to the 2π moved global minimum. Note: it is the other way around the SP

SP

2
1
2
π

moved global minimum. Note: it is the other way around the SP

SP

2
1
2
π

moved global minimum. Note: it is the other way around the SP

SP

2
1
2
π

moved global minimum. Note: it is the other way around the SP

SP

2
1
2
π

moved global minimum. Note: it is the other way around the SP

The used push and pull force is overwhelmingly simple. A scheme of the tilting for the on-site potential is shown in Figure 30. It pushes the first particle of the chain along its axis, and pulls the last particle into the same direction. All other particles are then moved by the springs between the particles. If one tilts the chain’s site-potential with this force, one gets a change of the stationary points along the NT; and at the end, for a large enough force, a sliding of the chain will be enforced, see Figure 31. That will be caused by a thermally activated transition between neighboring potential wells.

By the way, the two next still simpler directions, only push, or only pull [29] along the vectors (1,0,...,0) or (0,0,...,0,1) are not successful directions for an overall MEP of the chain. In the first case, the corresponding NT finds a way to the SP

SP

1
lb
1
lt
2
π

moved minimum iMin2; however, then it goes wrong anywhere into the mountains of the PES. It does not cross the SP

SP

1
lt
1
lb
2
π

moved minimum. In the second case, the corresponding NT finds a way to the other valley of the SP

SP

1
lb
1
lt
2
π

moved minimum iMin1; however, then it also goes wrong anywhere into the mountains. It does not cross the SP

SP

1
lt
1
lb
2
π

moved minimum. Both NTs also do not cross the SP

SP

in the center of interest here. The two directions do not belong to the small channel for successful ways, compare the brown curves in Figure 15.
7 Conclusion

Recently, experiments are done with laser-cooled and trapped ions for insights into friction processes [23,24,49, 86–88]. The systems try to emulate the FK model (1) for a small number N, where the chain of the interesting particles slides under an external force over the fixed rigid sinusoidal potential. The FK model (1) is not realistic in every detail. But it is sufficiently complex for tests of basic concepts [89]. Thus, any theoretical work to better understand such experiments is useful.

The PES (1) is given by an easy formula of the FK model. We can execute all calculations of NTs which determine the properties of the model. For comparison and confirmation we controlled the results of NT calculations by usual minimization procedures of the Mathematica program system because the PES of the FK model (1) is a usual surface where the known minimization procedures work. NTs are especially appropriate to the driven FK model by a tilting force. Of course, one can possibly find the existence of an LEP through the PES without the theory of NTs. One has simply to do an optimization for the global and intermediate minimums, and the SPs in between (if one is able to find these structures). However, an NT which follows more or less the LEP gives the direction of the tilting which can move the chain through this path.

An interesting aspect of the example with \( N = 23 \) particles is that usually not single particles form an anti-kink, a compression of a region of the chain. No, groups, like sets of triplets are involved in one step from a lower state to a higher one, and vice versa. Where two particles of the triplet stay in their well but the third particle moves over the top of the sinusoidal potential. Of course, this observation depends on the misfit parameter of 2/3 used here.

NTs allow us to drive them in very different directions over the PES. The standard direction \((1,\ldots,1)^T\) is physically well understandable. It would cause a washboard potential. However, beginning with the case \( N = 5 \) of the FK model [14], the standard direction is not a successful direction for a tilting with a low force. Our used directions deviate from the standard one. The corresponding valleys on the corrugated PES, which may also be very curvilinear, are better to follow by NTs which are adapted to the situation. So we work with a kind of tilting which concerns only parts of the chain with different weights. A possibly practicable case is the pure push and pull direction, \((1,0,\ldots,0,1)^T\), see Figure 30. The push and pull force at the ends allows the different atoms to individually move by their spring forces, but not collectively by an equal force for all. If one atom surmounts its top of the site-up potential then another can relax and can transmit its energy to the former one. Such better directions of a tilting allow that individual valleys of the PES open, and so optimal forces can be gotten. Perhaps experimental workers can construct an experiment where such optimal forces are applied to the chain.

This paper treats the ‘static’ PES of the 23-dimensional FK-chain. Additionally we look for a ‘step by step-series’ of tilted ‘static’ effective PESs under an assumed external force. The amount of the force is even increased step by step. The tilting changes the barriers of the original PES. This is the information which we generate and discuss here. Which kind of dynamics the chain develops if it is really tilted, this is not discussed here. To study it would be a next step following the knowledge of the valley through the PES. But of course, the picture of changing barriers along a path for a movement may give already an impression what can happen.

This paper discusses a special chain with \( N = 23 \) atoms for a special misfit parameter, 2/3. In a following paper, we discuss different series of chains to different misfit parameters with the aim to test the possible length of the chain up to a ‘critical’ value where the theory above becomes questionable. We guess that the here found LEPs through the PES continue to exist up to very high dimensions, in the kind ‘global minimum \(\rightarrow\) pre-SP \(\rightarrow\) intermediate minimum \(\rightarrow\) post-SP \(\rightarrow\) global minimum moved by \(a_q\)’. However, it will be more and more difficult to find a corresponding search direction for a unique NT which follows the path.

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Author contribution statement

All the authors were involved in the preparation of the manuscript. All the authors read and approved the final manuscript.

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