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The Frenkel-Kontorova Chain

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Introduction

Newton trajectories[1] are used for the Frenkel-Kontorova model of a finite molecular chain. We put free-end boundary conditions. The chain is embedded in a side potential. Thus the model has two competing potentials and it has an interesting potential energy surface. We optimize stationary structures, and we search the lowest energy saddle points for a complete minimum energy path for a movement of the chain over the period of the on-site potential, a sliding of the chain over the substrate.[2,3]
Newton trajectories are an ideal tool to understand the driving of a Frenkel-Kontorova chain by external forces. For special directions of the external force, the corresponding Newton trajectory follows the minimum energy path through the potential energy surface. Such external forces can cause a sliding of the chain which may be named superlubricity.
If the tilting is set, then one is interested in barrier breakdown points on the potential energy surface for a critical tilting force named the static frictional force.

The Model

$\mathbf{x} = (x_1, .., x_N)^T$ is a linear chain of N discrete particles. The boundaries are free. A spring force acts with a force constant k between the particles. The spacing is a constant natural distance a_o of the particles. A fixed on-site potential with a periodicity of a_s acts on the particles. The sinusoidal potential mimics a rigid, not deformable substrate. The ratio a_o/a_s is named the misfit parameter. The Frenkel-Kontorova model is

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

We put the factor v=1. 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. and we will generally get another average spacing, $\tilde{a}_o$.

Example

For an example we set $N = 23$, and the two parameters of the chain are $a_s = 2\pi$, but $a_0 = 4/3\pi$. The misfit value is then 2/3.

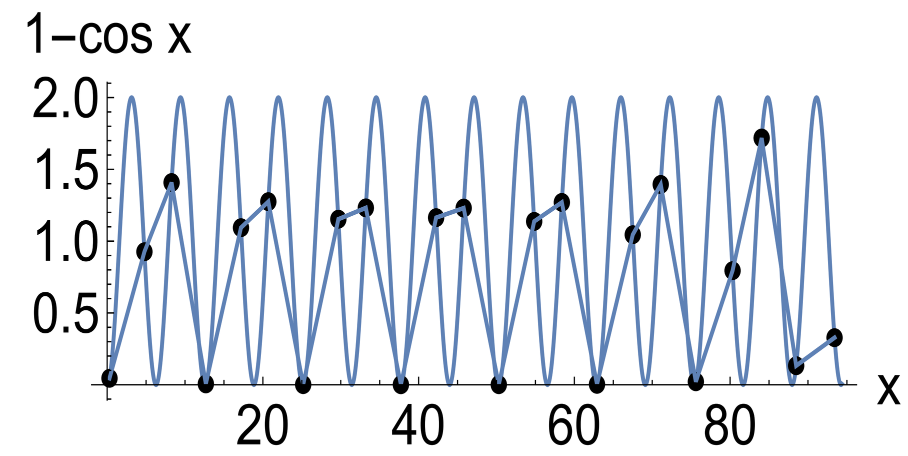

Fig. 1: Schematic picture of an asymmetric global minimum of the 23-particles chain.

The particles in Figure 1 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. Of course, here two mirror minima exist of the corresponding asymmetric kind.

Newton trajectories (NT)

In atomic force microscopy, a cantilever pulls a molecule with a given force in a defined direction. Such a tilting can be applied also to an Frenkel-Kontorova chain. Additionally to the two forces of the Frenkel-Kontorova model, we use an external, linear force in the ansatz. We name the resulting potential energy surface an effective potential energy surface

$$V_F(\mathbf{x}) = V(\mathbf{x}) - F\ (l_1, .., l_N)^T \cdot \mathbf{x}\ .$$

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

$$\nabla_{\mathbf{x}}\ V_F(\mathbf{x}) = \mathbf{g}(\mathbf{x}) - \mathbf{f} = \mathbf{0}\ .$$

One searches a point where the gradient of the original potential energy surface, $\mathbf{g}(\mathbf{x})$, has to be equal to the force, $\mathbf{f}$. The NT describes a curve of force-displaced stationary points of the tilted potential energy surface under a different load, F. Usually, the energy of a minimum can increase, but the energy of the next SP can be lower. This means that the barriers can become lower. At least, the barrier can disappear at a barrier breakdown point. To every NT belongs a barrier breakdown point, and for a special NT we have an optimal barrier breakdown point.[1,2,3]

By the way, following an NT is a method to search a next SP if a minimum is given, or vice versa.[1]

Example of Tilting

The tilting force used in our studies is mainly a push- and/or a pull-direction. It means the force acts only on the first particle, x_1 by $F\ (1, 0, .., 0)^T$, or on the last one by $F\ (0, ..., 0, 1)^T$.
Now we start with $N = 2$, $a_s = 2\pi$, $a_0 = 4/3\pi$, and $\mathbf{f}$=0.85 (1,0)^T.

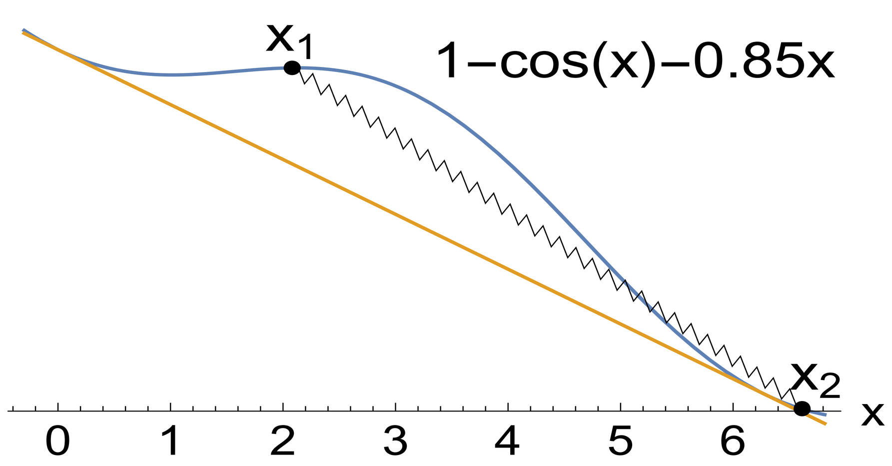

Fig. 2: 'Chain' with 2 atoms in relation to the tilted on-site potential.

The brown line in Figure 2 indicates the slope of the tilting. The spring length is extended to 4.53 (against 4.19 of the pure spring). Note that the location of x_1 on the on-site potential is only for an explanation. Here one can 'see' that the structure is short before starting to slide downhill the shoulders of the effective potential energy surface consistently.
The situation corresponds to a barrier breakdown point on the effective potential energy surface. The depinning of the chain starts.

Example of an NT

Again it is $N = 23$, and $a_s = 2\pi$, $a_0 = 4/3\pi$.

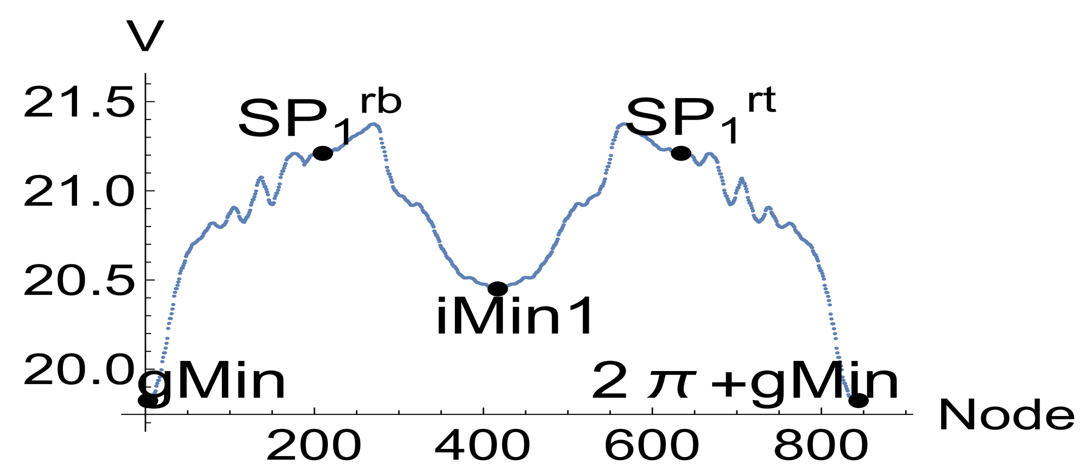

Fig. 3: Profile of an NT on the potential energy surface of a 23-chain.

Figure 3 shows a typical NT over the potential energy surface of a chain with 23 particles. It connects two global minima (gMin) with distance $a_s = 2\pi$ over two saddles (SP) and an intermediate (iMin). All stationary points are depicted by black bullets.
The NT is not smooth. It has some small spikes: they form turning points anywhere at the slope of the potential energy surface. On the potential energy surface two intermediates exist; they are separated by an SP of index two.[4] It plays a central role on the potential energy surface. The saddle point is a low summit[5] in the mountains.
Similar low energy pathways we found in chains to different misfit parameters, and with up to 101 particles.[6]

Example for an anti-kink

A new situation emerges for no misfit, thus misfit parameter=1. The periodicity of the springs of the chain, and of the side-up potential are equal. The ground state is a chain with particles down in the wells of the side-up potential, with zero energy. Under an external force, the chain can suffer by an anti-kink like in Figure 5. Here, the potential energy surface has a 'flat'-SP-pathway.[6]

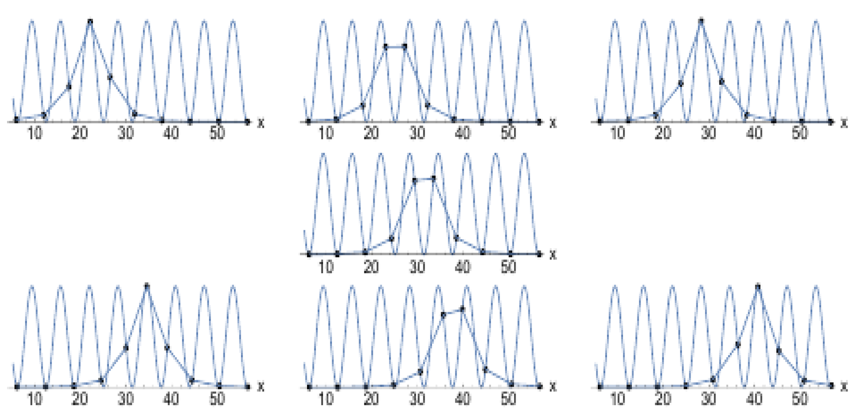

Fig. 5: Misfit=1 – the panels alternate SP$_1$ and iMin structures.

Figure 5 shows a 10-chain with misfit=1. The panels alternate consecutive SP$_1$ and iMin structures. The latter depict an anti-kink which moves through the chain. The 'SP'-path is quasi flat. Only the ascent to the first SP$_1$ needs a strong energy amount, and after the last SP$_1$, the path stronly descents back to zero energy, compare Figure 6.

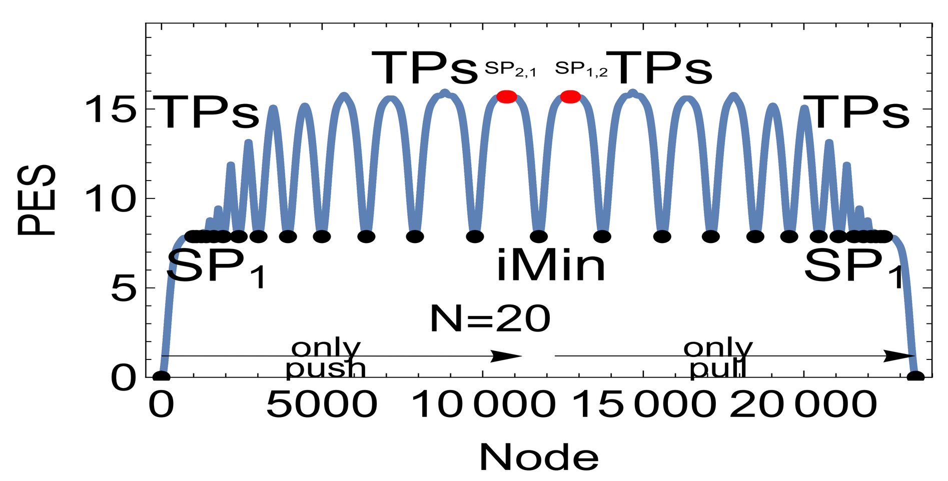

Fig. 6: Profile over an NT on the potential energy surface of a 20-chain.

Figure 6 shows the energy profile on the potential energy surface of an NT for the 20-chain with misfit=1. The alternating SP$_1$ and iMin structures form the quasi flat barrier. They are the lower spikes of the NT. They describe an anti-kink which moves through the chain on really equal level. However, the NT which explores the stationary points does not lead along the valley floor, it does not directly connect the consecutive saddle-sink sequence, but it escapes to very higher energies with turning points (TPs) at the top of the peaks, and additional SPs of index 2 and 1 (red points). The minimum energy path itself leads over all the black bullets.

References

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