

Newton Trajectories for the tilted Frenkel-Kontorova Model

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Supplementary Material

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1. Data of the discussed structures of the 23-atomic chain

1.1. a) *The 'left' minimum is at energy 19.824175.*

The structure is shown in the text.

Coordinates

0.3010 4.78629 8.2743 12.6753 17.1849
20.699 25.1744 29.6916 33.2206 37.7223
42.2472 45.7856 50.297 54.84 58.3925
62.908 67.4994 71.0919 75.6031 80.3176
84.0536 88.4852 93.4143

The 5 lowest eigenvalues are:

0.3565, 0.2293, 0.1675, 0.1132, 0.0000402.

The lowest eigenvector is

0.0309, 0.0600, 0.0987, 0.0851, 0.1543,
0.2454, 0.1913, 0.3163, 0.5759, 0.3015,
0.2499, 0.4041, 0.2325, 0.128, 0.1472,
0.0977, 0.0505, 0.0533, 0.0368, 0.0193,
0.0207, 0.0131, 0.0067

1.1. b) *The 'right' minimum is*

Coordinates

0.8314, 5.7595, 10.188, 13.9256, 18.6413,
23.1508, 26.744, 31.3368, 35.8509, 39.4036,
43.9479, 48.4581, 51.9966, 56.5227, 61.0232,
64.5523, 69.0706, 73.5450, 77.0593, 81.5701,
85.9700, 89.4589, 93.9452

Its structure is shown in the text.

1.2. The symmetric SP_1 between the two global minimums

Coordinates

0.324, 4.832, 8.346, 12.742, 17.313,
20.884, 25.349, 30.03, 33.728, 38.163,
43.046, 47.124, 51.202, 56.085, 60.520,
64.218, 68.898, 73.364, 76.935, 81.506,
85.902, 89.416, 93.924

Its energy is 19.96437. Its structure is shown in the text. Its first eigenvalues are: -0.0265, 0.0109, 0.0725, 0.1598. The negative eigenvector is not symmetric

0.1017, 0.1813, 0.3995, 0.2512, 0.2277,
0.4063, 0.2626, 0.2062, 0.3409, 0.2239,
0.1672, 0.2676, 0.1747, 0.1254, 0.1945,
0.125, 0.0861, 0.1289, 0.0797, 0.0512,
0.0713, 0.0396, 0.0204

1.3. a) *BBP on the NT to direction $(1, \dots, 1)^T$*

The left BBP point is at energy 19.88 with the gradient norm 0.087.

0.372, 4.907, 8.446, 12.794, 17.349,
20.894, 25.307, 29.873, 33.428, 37.865,
42.445, 46.016, 50.459, 55.072, 58.679,
63.112, 67.801, 71.510, 75.881, 80.695,
84.660, 88.772, 93.59

1.3. b) *The right BBP point*

It is at energy 19.8725 with the gradient norm 0.08.

0.657, 5.473, 9.579, 13.552, 18.378,
22.761, 26.461, 31.156, 35.606, 39.198,
43.812, 48.269, 51.826, 56.406, 60.856,
64.397, 68.963, 73.389, 76.921, 81.476,
85.839, 89.359, 93.886

1.4. A second SP_1 between the two minimums

Coordinates

0.782, 5.675, 9.997, 13.777, 18.494,
22.862, 26.465, 31.040, 35.249, 38.82,
43.291, 47.124, 50.957, 55.428, 58.999,
63.207, 67.783, 71.386, 75.754, 80.470,
84.251, 88.573, 93.466

Its energy is 20.1993. Its symmetric structure is shown in the text. The lowest eigenvalues are 0.1814, 0.0756, 0.0488, -0.0278.

The negative eigenvector is

0.025, 0.0434, 0.0987, 0.0737, 0.0768,
 0.1539, 0.1361, 0.1543, 0.3204, 0.2485,
 0.2916, 0.5674, 0.2916, 0.2485, 0.3204,
 0.1543, 0.1361, 0.1539, 0.0768, 0.0737,
 0.0987, 0.0434, 0.025

1.5. The SP_2 in between

It is at an energy of 20.2139 units.

0.6289	5.4070	9.4167	13.4345	18.2154
22.4039	26.1912	30.8502	34.9731	38.6923
43.2493	47.1371	51.0117	55.5652	59.2863
63.4005	68.0531	71.8323	76.0233	80.7994
84.8035	88.8271	93.6102		

Its structure is shown in the text.

Its lowest eigenvalues are 0.1924, 0.1002, 0.0067, -0.0366, -0.07249.

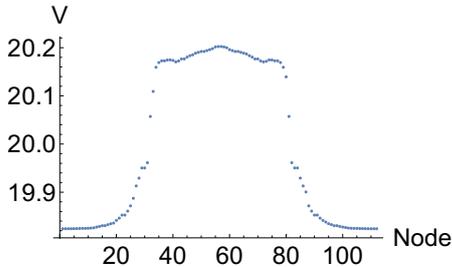


Figure 1. Energy profile over a singular NT connecting the two asymmetric global minimums over a maximum which corresponds to the symmetric SP_2 .

2. Programming

The used parameter of the Fortran program:

N=23, Eps=1.0*E-06, ItMax=7.

Eps is the convergence criterion of the corrector step.

ItMax is the maximal number of corrector steps.

The norm of the corrector step is maximally 1.0. The corrector sometimes proposes larger steps: they are shorten automatically to 1.0 norm. (Nevertheless the program sometimes goes wrong.)

The number L of nodes was varied, from 65 up to some hundreds, for different aims and versions of the program. (It should be $L=2 \bmod 7$ for an output for the Mma program.) Usually the results are very similar, independent on the number of nodes.

Because for special points the Mma optimization and the Fortran program for NTs result in identical values, one can assume that both are correct; as long as the function and the gradient are treated. Our conclusions are arguable.

3. Cooperation

A set of further SPs was detected. They are reported in a further paper. We would like to exchange the data with interested workers. It concerns, as well, the programs (Fortran, and Mathematica).