ATOMIC SCALE ENGINES: TAKING A TURN*

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We investigate a new approach which has been recently introduced to construct microscopic engines whose main characteristic is the possibility to determine *dynamically* the direction of motion. The approach is based on the transformation of the supplied energy into directed motion through a dynamical competition between the intrinsic lengths of the moving object and the substrate. The engines are able to move translationally or rotationally and can perform useful functions such as pulling of a cargo. We discuss possible realizations and introduce some ingredients, such as turns and switches, important for creating a microscopic 'railway system.'

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1. Introduction

When Feynman made his visionary predictions concerning nanoscale technology almost 40 years ago [1], nobody really believed that the handling of single atoms and molecules would become so widespread in science as it is today [2]. A major step forward has been made about 20 years ago, when the window to the 'nanosize world' has been opened with the invention of scanning-tunnelling [3] and atomic force microscopies [4]. These techniques have radically changed the way we view and interact with nanoscale objects making possible their imaging [5,6] and, even more striking, their manipulation [6–9]. Nevertheless, the important challenge still remains to further

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'tame' molecules and make them perform useful functions, such as transportation. Despite a growing interest in atomic scale engines, such as biological motors [10,11], ratchet systems [10,12–15], molecular rotors [7–9,16], and molecular machinery in general [17], a real breakthrough concerning the construction of a man-made nanoscale counterpart of the 'steam locomotive' and its corresponding 'railway system' has not occured yet. This has mainly been due to the fact that we still miss the crucial link of how to transform energy into directed motion on this scale.

Recently, we have proposed the basic principles that can make such an engine possible [18]. The main advantages of this engine are:

- the directionality of motion is determined *dynamically* and does not require any spatial asymmetry of the moving object or of the substrate,
- the engine is powerful enough to allow for the transportation of a cargo,
- the same concept applies for both translational and rotational motions, and
- the velocity obtained can be varied over a wide range, independent of the direction.

Here, we discuss some ingredients which help to construct a 'railway system' for the engine to allow for taking turns and crossing tracks.

The Article is organized as follows: in Section 2 the specific model system is introduced. In Section 3 we present a few selected scenarios, and we conclude in Section 4.

2. Model

The proposed engine consists in general of two parts: the substrate and the moving object. Achieving motion of the engine is based on the dynamical competition between the two intrinsic lengths of the substrate and the object. This dynamical competition is used to transform initially fed energy into directed motion. To exemplify this concept, we use below a simple model system of a chain [the moving object] in a periodic potential [the substrate], namely a Frenkel–Kontorova type model [19]. We would like to emphasize that this choice as an example is solely motivated by the simplicity of the model rather than by experimental requirements. In particular, it is not necessary for the particles to be single atoms and the springs are not necessarily single chemical bonds, different from the original Frenkel–Kontorova model. The sole purpose of the model system is to address in a simple and intuitive manner the following questions:

(a) What is the minimal size of the engine?

(b) How are the direction and velocity of the motion determined?

(c) How powerful is the engine?

(d) How to make the engine performing a turn? and

(e) How to construct devices such as switches which help to cross tracks and directions?

The issue of possible physical realizations of the model will be addressed towards the end of the article.

In the model system the substrate is taken as an isotropic surface, and the moving object as a chain of N identical particles on the surface. Each particle i has a mass m and is located at coordinate x_i. For simplicity, we restrict the first part of the discussion to translational motion in one dimension; Fig. 1(a) displays a sketch of the model geometry for $N = 3$.

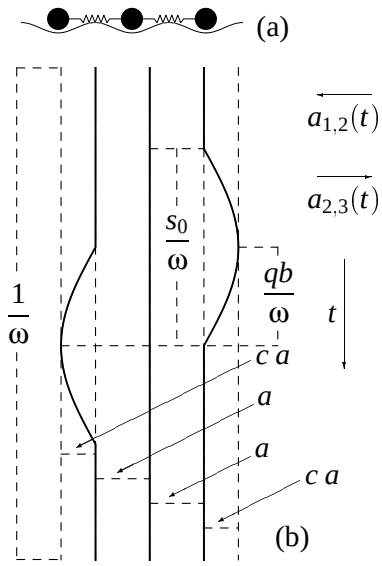

Fig. 1. (a) Sketch of the geometry of the example engine, showing the surface potential $\Phi(x)$ and the chain with $N = 3$ particles. (b) Changing the free rest lengths $a_{i,i+\delta_i}(t)$; the lengths $a_{1,2}(t)$ and $a_{2,3}(t)$ as a function of time t are shown. The parameters are: The wave vector $q = 1/(5b)$, the peak amplitude $c = 7/10$, and the peak width $s_0 = 4/10$.

The N equations of motion read as

$$m\ddot{x}_i + \eta\dot{x}_i + \frac{\partial\Phi(x_i)}{\partial x_i} + \sum_{\delta_i} \frac{\partial\Psi(x_i - x_{i+\delta_i})}{\partial x_{i+\delta_i}} = 0 \qquad i = 1, \ldots, N. \tag{1}$$

The second term in Eq. (1) describes the dissipative interaction [friction] between the particles and the substrate and is proportional to their relative velocities with proportionality constant η. The static interaction between the particles and the surface is represented by the periodic potential

$$\Phi(x) = -\Phi_0 \cos\left(\frac{2\pi x}{b}\right) \tag{2}$$

with periodicity b. Concerning the inter-particle interaction, we take a nearest neighbor harmonic interaction

$$\Psi(x_i - x_{i+\delta_i}) = \frac{k}{2} \left[|x_i - x_{i+\delta_i}| - a_{i,i+\delta_i}(t)\right]^2 \tag{3}$$

with free equilibrium rest lengths $a_{i,i+\delta_i}(t)$ [$i + \delta_i = i \pm 1$ denotes the nearest neightbors of particle i]. Different from the original Frenkel–Kontorova model, the $N-1$ free equilibrium rest lengths $a_{i,i+\delta_i}(t)$ are not constant, but do depend both on the bond's position, specified by the indices $i, i+\delta_i$, and on time t. The time dependent modulation of $a_{i,i+\delta_i}(t)$ opens a simple and straightforward mechnism to pump energy into the system. In general, if the lengths $a_{i,i+\delta_i}(t)$ are changed in an uncorrelated fashion, or when using an inproper spatial and temporal correlation for the $a_{i,i+\delta_i}(t)$ for different bonds at different times, a diffusive motion of the chain results. Nevertheless, there are cases in which energy is pumped into the system in a specific manner that provides spatially and temporally correlated changes of the $a_{i,i+\delta_i}(t)$, so that the dynamical local competition between the periodicity b and the rest lengths $a_{i,i+\delta_i}(t)$ can induce a *directed* motion of the chain.

3. Results

Without specifing the dependence of the rest lengths $a_{i,i+\delta_i}(t)$ on the bond's position $i, i+\delta_i$ and time t, the above approach describes a whole family of possible small scale engines. In the following we restrict ourselves to a certain choice of $a_{i,i+\delta_i}(t)$, that leads to an engine having a minimum size of as small as $N = 3$ particles. The position and time dependent rest lengths $a_{i,i+\delta_i}(t)$ are chosen as

$$a_{i,i+\delta_i}(t) = a \left[1 + \alpha\left(q x_{i,i+\delta_i} + \omega t\right)\right], \tag{4}$$

resulting in a specific spatial–temporal correlation between the lengths of different bonds given by the combined argument $qx_{i,i+\delta_i} + \omega t$. Here, $x_{i,i+1} = ib$ and $x_{i,i-1} = x_{i-1,i}$ are the relative positions of the bonds between particles i and $i \pm 1$ [*i.e.* $a_{i,i-1}(t) = a_{i-1,i}(t)$]. The length a, the wave vector q, and the driving frequeny ω are parameters. The function $\alpha(s)$ has a periodicity of 1 such that $\alpha(s+1) = \alpha(s)$ for all s, and is chosen as

$$\alpha(s) = \begin{cases} c \sin(\pi s / s_0) & \text{for } 0 \le s \le s_0 \\ 0 & \text{for } s_0 \le s \le 1 \end{cases} , \tag{5}$$

with the peak width s_0 and the peak amplitude c being parameters. In Fig. 1(b) shown are 10 snapshots of the time dependence of the free rest lengths $a_{i,i+\delta_i}(t)$ for a chain with $N = 3$ particles, displaying the meaning of the parameters q, s_0, and c.

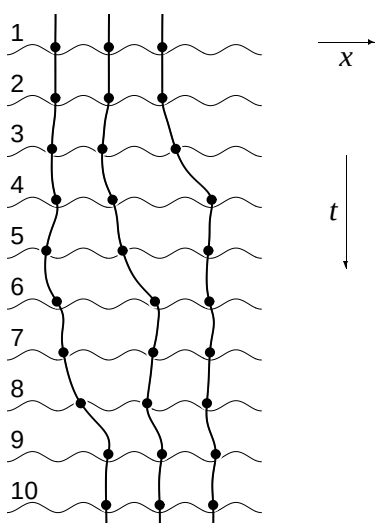

Fig. 2. Motion of the chain sketched in Fig. 1(a); the positions x_i of the particles as a function of time t are shown. The large disks indicate the particles' position in relation to the surface potential in the 10 numbered snapshots in time intervals of $5b/(2\pi)\ \sqrt{m/\Phi_0}$. The time $25b/\pi\ \sqrt{m/\Phi_0}$ of a full oscillation of $a_{i,i+\delta_i}(t)$ and hence of a single step of length b to the right is shown. The parameters are: The misfit between the minimum rest length of the inter-particle potential and the potential period $a/b = 11/10$, the dissipation constant $\eta = 16\pi/(10b)\ \sqrt{\Phi_0 m}$, the inter-particle potential strength $k = [(2\pi)/b]^2\ \Phi_0$, the driving frequency $\omega = \pi/(25b)\ \sqrt{\Phi_0/m}$, the wave vector $q = 1/(5b)$, the peak amplitude $c = 7/10$, and the peak width $s_0 = 4/10$.

The motion of the complete engine consisting of a chain and a surface, as sketched in Fig. 1(a), is shown in Fig. 2 in 10 snapshots. Despite the fact that there is no external force acting on the chain, a directed motion of the chain to the right results [note that the 10^{th} snapshot is equivalent to the 1^{st} as the chain moved by a length b to the right]. It is important to note that the symmetry in the system is broken *dynamically*, as a result the direction of the motion is *dynamically* determined and is solely given by the bond whose rest length increases first, starting when the particles are located at the minima of the surface potential [the right one in Fig. 2]. In general, for more than two bonds, the 'excitation' has to propagate opposite to the desired direction of motion, starting at the particle that is frontmost. This can be achieved by using $a_{i,i+\delta_i}(t) = a\,[1+\alpha(qx_{i,i+\delta_i}+\omega t)]$ for a motion in positive and $a_{i,i+\delta_i}(t) = a\,[1+\alpha(qx_{i,i+\delta_i}-\omega t)]$ for a motion in negative x-direction [note the different signs in front of ω]. Therefore, the motion can be easily controlled; in particular the direction can be chosen independent of velocity, and the motion can be stopped and restarted, either in the same or in the opposite direction.

For the above choice of $a_{i,i+\delta_i}(t)$ and for not too high frequencies [up to a maximum frequency $\omega_{\max} \approx \pi/(25b)\,\sqrt{\Phi/m}$, keeping the other parameters fixed], the engine's velocity v is proportional to the driving frequency ω through $v = b\omega$, so that the maximum velocity is given approximately by $v_{\max} \approx \pi/25\,\sqrt{\Phi/m}$. For higher driving frequencies the motion gets first irregular and finally diffusive, loosing its directionality.

The wave vector q determines the correlation between the different rest lengths. A choice of $q = 1/(5b)$ as used in Figs. 1 and 2 turns out to yield a large maximum velocity and a 'powerful' engine for $N = 3$. A simple measure for how powerful this engine is, can be determined by a straightforward procedure [20], where the chain moves against a constant force experienced by each particle. The chain with parameters as in Figs. 1 and 2 is able to move against a constant force of up to $F_{\max} \approx \Phi_0/b$, maintaining the velocity $b\omega$. For higher opposing forces, the chain remains at its initial location, and for even higher opposing forces, the chain moves with the force. It is important to note that the maximum possible opposing force depends sensitively on the parameters, in particular on the constant c and the wave vector q.

Another possible intuitive way to measure how powerful the engine is, is to let the chain transport a cargo of N' additional inactive particles attached at its end with the same inter-particle potential $\Psi(x_i - x_{i+\delta_i})$, but with a *constant* rest length a. It turns out that, depending on the choice of parameters, a chain of N particles is able to transport up to a maximum of $N'_{\max} \approx N/2$ additional inactive particles and hence up to about half its own weight on an isotropic surface. As an example, in Fig. 3 shown is a

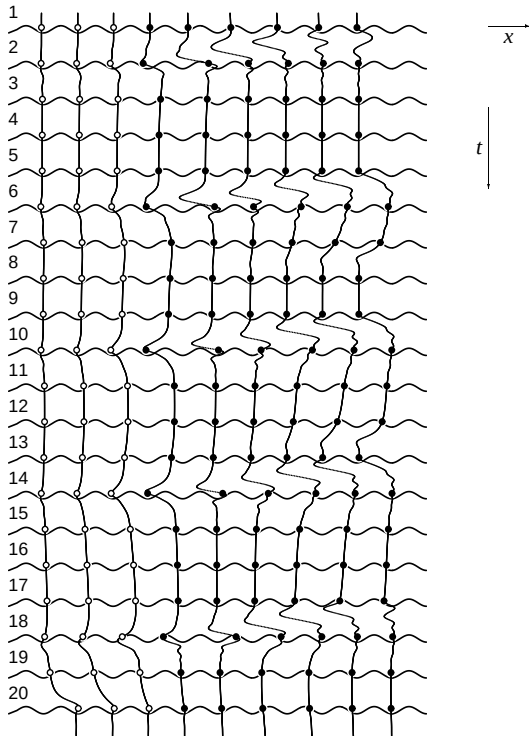

Fig. 3. Motion of the chain with $N + N' = 9$ particles; the positions x_i of the particles as a function of time t are shown. The large disks indicate the particles' position in relation to the surface potential in the 20 numbered snapshots in time intervals of $25b/(4\pi)\ \sqrt{m/\Phi_0}$. The chain consists of an active part containing $N = 6$ particles shown as full disks [*i.e.* five active bonds], and a cargo of $N' = 3$ particles shown as open disks [*i.e.* four inactive bonds]. The time $125b/\pi\ \sqrt{m/\Phi_0}$ of five full oscillations of $a_{i,i+\delta_i}(t)$ is shown, corresponding to a single step of length b to the right. The parameters are identical to those in Fig. 2, except the wave vector $q = 1/(20b)$ and the peak width $s_0 = 1/10$.

chain of in total $N + N' = 9$ particles, composed of an actice part of $N = 6$ particles and a cargo of $N' = 3$ particles. As can be seen in the figure, after five full oscillation of $a_{i,i+\delta_i}(t)$, the active part consisting of five active bonds has pulled the inactive cargo one potential period b to the right. After that, the whole process starts over again. Here, due to the presence of the cargo, the velocity of the total entity is reduced to $b\omega/5$.

Two important questions are (a) the influence of the shape of the 'excitation' $\alpha(s)$, which is sinusodial in our case [*cf.* Eq. (5)], and (b) the influence of noise, since Eq. (1) is deterministic. One should note that, as long as the 'excitation' is approximately trapezoidal, a proper choice of driving fre-

quency ω and wave vector q results in a directed motion. Similarly, as long as the thermal energy $k_{\mathrm{B}}T$ is much smaller than the energy scale Φ_0, the engine's motion is hardly influenced by noise. If the fluctuations become larger, the motion gets erratic. Finally, for $k_{\mathrm{B}}T \gg \Phi_0$, the motion looses completly its directionality and becomes diffusive.

So far, our discussion has been restricted to a linear one-dimensional system. However, one of the main advantages of the above concept is that (a) it can easily be applied to other types of motion and (b) it can be generalized to higher dimensionalities. This is mainly due to the absence of any static asymmetry in the system. Let us first briefly mention the case of other types of motion. An engine that performs *rotational* motion can be achieved by treating the coordinates x_i as angular coordinates $x_i \in [0, \ell)$ on a circle of circumference of length $\ell = nb$ with n integer, and periodic boundary conditions. Such a 'wheel' can rotate either clockwise or counterclockwise. We will not further discuss this possibility, for a detailed description of rotational motion see [18].

Concerning the application to a higher dimensionality, we consider a chain moving on a two-dimensional surface by replacing in Eq. (1): (a) the 1D coordinates x_i by 2D ones $\vec{x}_i$, (b) the 1D partial derivations $\partial/\partial x_i$ by 2D gradients $\vec{\nabla}_{\vec{x}_i}$, (c) the 1D surface potential $\Phi(x)$ in Eq. (2) by a 2D counterpart

$$\Phi(\vec{x}) = -\Phi_0 \cos\left(\pi \frac{\vec{x}^{(1)} - \vec{x}^{(2)}}{b}\right) \cos\left(\pi \frac{\vec{x}^{(1)} + \vec{x}^{(2)}}{b}\right) \tag{6}$$

[$\vec{x}^{(i)}$ denotes the i-th component of the vector $\vec{x}$], and (d) the 1D interparticle potential $\Psi(x_i - x_{i+\delta_i})$ by the 2D counterpart

$$\Psi(\vec{x}_i - \vec{x}_{i+\delta_i}) = \frac{k}{2}\left[\left|\vec{x}_i - \vec{x}_{i+\delta_i}\right| - a_{i,i+\delta_i}(t)\right]^2, \tag{7}$$

where $\left|\cdot\right|$ denotes vector length. Using the same form for $a_{i,i+\delta_i}(t)$ as in the case of 1D, Eqs. (4), (5), the chain can be moved along the 2D surface, see Fig. 4. The existance of a working 2D version of the model system opens many possibilities. One example is the possibility to construct a complex atomic scale 'car' by connecting six chains in such a way that they constitute an array of 3×3 particles connected by 12 bonds. By exciting three parallel chains coherently, this 'car' can be moved both forward and backward as well as left and right, so that it can be driven *freely* over the surface [18].

A further striking modification is to built a kind of microscopic 'railway system.' The important ingredients needed for this are (a) parts that enable a straight motion [as shown in Fig. 4], (b) parts making the engine perform turns, and (c) switches that allow for crossing tracks and directions.

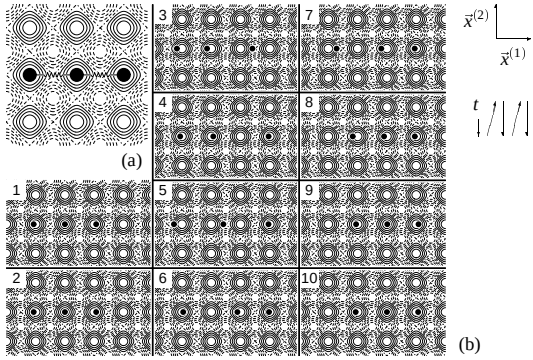

Fig. 4. (a) Sketch of the 2D atomic scale engine, a chain of $N = 3$ particles. The surface potential $\Phi(\vec{x})$ is indicated by equipotential lines shown for $\Phi(\vec{x}) = n\Phi_0/5$ with $-5 \leq n \leq 5$ integer, which are continuous for $\Phi(\vec{x}) < 0$, dashed for $\Phi(\vec{x}) > 0$, and dashed-dotted for $\Phi(\vec{x}) = 0$. (b) Motion of the chain sketched in (a); the disks indicate the particles' position in relation to the surface potential in the 10 numbered snapshots in time intervals of $5b/(2\pi)\sqrt{m/\Phi_0}$. The time $25b/\pi\sqrt{m/\Phi_0}$ of a full oscillation of $a_{i,i+\delta_i}(t)$ and hence of a single step of length b to the right is shown. The parameters are identical to those in Fig. 2.

To obtain a simple example of a turn, we rewrite the potential given by Eq. (6) using polar coordinates r and ϕ and replace in Eq. (6) $\vec{x}^{(1)}$ by $\chi r/(\kappa/2\pi)$ and $\vec{x}^{(2)}$ by $b(\phi - \pi/2)/(2\pi/\kappa)$. This results in

$$\begin{aligned} \Phi'(\vec{x}) \;&=\; -\Phi_0 \;\cos\left(\pi\;\left[\frac{\chi r}{\kappa b/(2\pi)} - \frac{\phi - \pi/2}{2\pi/\kappa}\right]\right) \\ &\quad \times \cos\left(\pi\;\left[\frac{\chi r}{\kappa b/(2\pi)} + \frac{\phi - \pi/2}{2\pi/\kappa}\right]\right), \end{aligned} \tag{8}$$

where the parameter κ is an even integer denoting the 'order' of the turn, *i.e.* the number of minima along a circle with circumference κb [*i.e.* radius $\kappa b/(2\pi)$]. The parameter χ is chosen as the closest integer to $\kappa/(2\pi)$, so that the width of the circular valley is approximately equal to b. An example of the potential $\Phi'(\vec{x})$ in Eq. (8) is shown in Fig. 5. Using the same mechanism as in Fig. 4, the chain can be moved inside the valley around the center of the circle. By using, for example, only one half or one fourth of the total circle and connecting this part with other (straight) parts, one can construct turns by π or $\pi/2$.

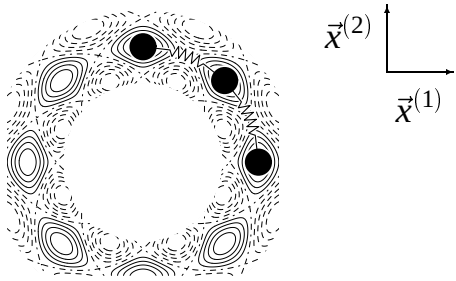

Fig. 5. Sketch of the 2D atomic scale engine, a chain of $N = 3$ particles, taking a turn of 'order' $\kappa = 8$ [$\chi = 2$]. The surface potential $\Phi'(\vec{x})$ is indicated by equipotential lines shown for $\Phi'(\vec{x}) = n\Phi_0/5$ with $-5 \leq n \leq 5$ integer, which are continuous for $\Phi'(\vec{x}) < 0$, dashed for $\Phi'(\vec{x}) > 0$, and dashed-dotted for $\Phi'(\vec{x}) = 0$.

Using a similar idea one can construct a switch. Combining two potentials, one of which is given by Eq. (8) and the other one of the same form but translated by $\vec{x}_0$ with $\vec{x}_0^{(1)} = \kappa b/\pi$ and $\vec{x}_0^{(2)} = 0$, we obtain

$$\Phi''(\vec{x}) = \begin{cases} \Phi'(\vec{x}) & \text{for } \vec{x}^{(1)} \leq \kappa b/(2\pi) \\ \Phi'(\vec{x} - \vec{x}_0) & \text{for } \vec{x}^{(1)} > \kappa b/(2\pi) \end{cases} . \tag{9}$$

The potential $\Phi''(\vec{x})$ defines an acute crossing, as shown in Fig. 6. Modifying locally the potential by adding a perturbative barrier of a Gaussian shape at the positions indicated by the arrows in Fig. 6 introduces the possibility that this acute crossing can work as a switch: One either forces the chain entering the crossing to continue towards the left exit [Fig. 6(a)] or towards the right exit [Fig. 6(b)]. It is worthwhile to note that without any perturbation, a chain entering from the left, as shown in Fig. 6, will leave through the right exit, whereas a chain entering from the right will leave through the left exit. This is quite similar to the case of rectangular crossings as given by the four-fold symmetry of Eq. (6), where, however, a local modification of the potential is not enough to control the further motion of the chain.

By combining all three ingredients (the straight parts, the turns and the switches) together in a suitable way, one might be able to construct a broad range of track geometries. Examples include closed loops, 8-shaped geometries, and so on.

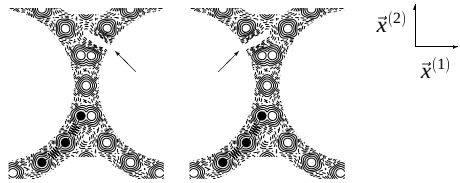

Fig. 6. Sketch of the 2D atomic scale engine, a chain of $N = 3$ particles, in the presence of a switch constructed by two turns of 'order' $\kappa = 18$ [$\chi = 3$]. The surface potential $\Phi''(\vec{x})$ is indicated by equipotential lines shown for $\Phi''(\vec{x}) = n\Phi_0/5$ with $-5 \leq n \leq 5$ integer, which are continuous for $\Phi''(\vec{x}) < 0$, dashed for $\Phi''(\vec{x}) > 0$, and dashed-dotted for $\Phi''(\vec{x}) = 0$. The switch is in the state 'left' in (a), and in the state 'right' in (b). The location of the local perturbation is indicated by the arrows.

4. Conclusions

As a conclusion, we would like to reemphasize that the choice of a chain on a substrate as the example engine has been motivated solely by the simplicity of the model system rather than by experimental requirements. One important feature of the concept introduced in [18] is that it does not impose any specific length or time scales. This means that it is applicable not only for an engine on an atomic scale, but also for mesoscopic or even macroscopic sizes. Hence, the basic concept of competing lengths is more general than presented in [18] and here and might be applicable in a wide range of situations.

A possible realization on an atomic or mesoscopic scale might be feasible by constructing the moving object using nanosize clusters [the 'particles'] and photochromic molecules [the 'bonds']. The time dependence of the rest lengths, which is a crucial part of the concept, can be provided by individually controlling the 'bonds' by light induced conformational changes of the chromophors. Using different chromophores which respond to different wavelengths should allow to specifically excite 'bonds' at chosen locations at given times. In this proposed realization, the surface corrugation might be feasible by nanolithography. Therefore, we believe that the current concept is simple and robust enough so that it can be realized in actual experiments using already existing techniques. Such an atomic scale engine, when realized experimentally, will be a real achievement in the field of nanotechnology by providing new ways to manipulate molecules and clusters.

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