Atomic Scale Engines: Cars and Wheels

Markus Porto, Michael Urbakh, and Joseph Klafter
School of Chemistry, Tel Aviv University, 69978 Tel Aviv, Israel
(Received 16 December 1999)

We introduce a new approach to build microscopic engines on the atomic scale that move translationally or rotationally and can perform useful functions such as the pulling of a cargo. Characteristic of these engines is the possibility to determine *dynamically* the directionality of the motion. The approach is based on the transformation of the fed energy to directed motion through a dynamical competition between the intrinsic lengths of the moving object and the supporting carrier.

PACS numbers: 66.90.+r, 45.40.Ln, 87.16.Nn

The handling of single atoms and molecules has become widespread in science [1], but the challenge still remains to further "tame" them and make single molecules perform useful functions. Nanoscale technology has been predicted almost 40 years ago [2], but in spite of a growing interest in atomic scale engines, such as biological motors [3,4], ratchet systems [3,5–7], molecular rotors [8–11], and molecular machinery in general [12], a real breakthrough concerning the construction of a man-made nanoscale counterpart of the "steam engine" has not occurred yet. This has mainly been due to the fact that we still miss the crucial link of how to transform energy to directed motion on this scale.

In this Letter we propose possible basic principles of such an engine. The main advantages of this novel approach are (a) the same concept applies for both translational and rotational motions, (b) the directionality of motion is determined *dynamically* and does not require spatial asymmetry of the moving object or of the supporting carrier, (c) the velocity obtained can be varied over a wide range, independent of the direction, and (d) the engine is powerful enough to allow for the transportation of a cargo.

The proposed engine consists in general of two parts: the supporting carrier and the moving object. Achieving motion of the engine is based on dynamical competition between the two intrinsic lengths of the carrier and the object. This competition is used to transform initially fed energy to directed motion. To exemplify the concept, we use below a *simple* model system of a chain in a periodic potential, namely, a Frenkel-Kontorova-type model [13]. But 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, the particles are not meant to be single atoms and the springs are not meant to be single chemical bonds. The sole purpose of the model system is to address in a simple 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? The important questions of possible physical realizations will be addressed towards the end of this Letter.

In the model system, as already mentioned, the supporting carrier 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 $N = 3$. The N equations of motion read as

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

The second term in Eq. (1) describes the dissipative interaction (friction) between the particles and the surface 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 $\Phi(x) = -\Phi_0\cos(2\pi x/b)$ with periodicity b. Concerning the interparticle interaction, we take a nearest neighbor harmonic interaction $\Psi(x_i - x_{i+\delta_i}) = (k/2)[|x_i - x_{i+\delta_i}| - a_{i,i+\delta_i}(t)]^2$ with free equilibrium rest lengths $a_{i,i+\delta_i}(t)$ ($i + \delta_i = i \pm 1$ denotes the nearest neighbors of particle i). The $N - 1$ rest lengths depend both on the bond's position specified by the indices $i, i + \delta_i$ and on time t. We demonstrate that if energy is pumped into the system in a specific manner that provides spatially and temporally correlated changes of the lengths $a_{i,i+\delta_i}(t)$, 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.

Without specifying the dependence of the rest lengths $a_{i,i+\delta_i}(t)$ on the bond's position and time, the above approach describes a whole family of atomic scale engines. In the following we restrict ourselves to a certain choice for $a_{i,i+\delta_i}(t)$ that results in 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 $a_{i,i+\delta_i}(t) = a[1 + \alpha(qx_{i,i+\delta_i} + \omega t)]$, resulting in a certain fixed spatial and temporal correlation between the lengths of different bonds. 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

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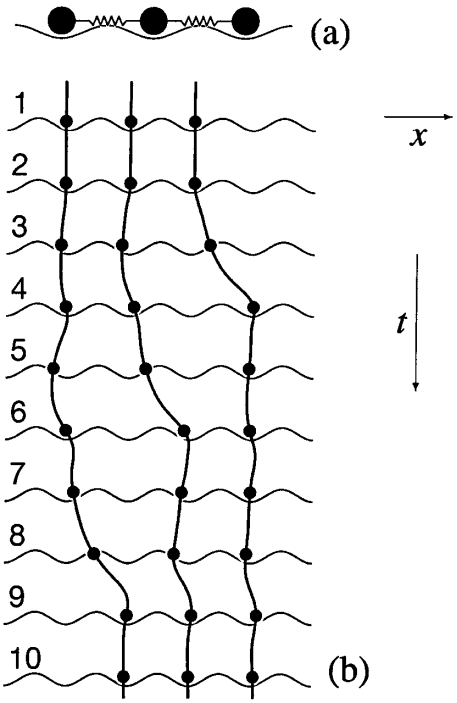

FIG. 1. (a) Sketch of the geometry of the example engine showing the surface potential $\Phi(x)$ and the chain with $N = 3$ particles. (b) Motion of the chain sketched in (a); the position x_i of the particles as a function of time t is shown. The large disks indicate the particles' position in relation to the surface potential in the ten 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 interparticle potential and the potential period $a/b = 11/10$, the dissipation constant $\eta = (16\pi/10b)\sqrt{\Phi_0 m}$, the interparticle 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 amplitude $c = 7/10$, and the peak width $s_0 = 4/10$.

$i \pm 1$. The length a, the wave vector q, and the driving frequency 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 $\alpha(s) = c\sin(\pi s/s_0)$ for $0 \le s \le s_0$ and $\alpha(s) = 0$ for $s_0 \le s \le 1$, with s_0 and c being parameters. Shown in Fig. 1(b) are ten snapshots of the motion for a complete step of length b to the right for the engine sketched in Fig. 1(a) (note that the 10th snapshot is equivalent to the 1st as the chain moved by a length b to the right). The direction of the motion is *dynamically* determined and solely given by the bond whose rest length increases first, starting when the particles are in the minima of the surface potential [the right one in Fig. 1(b); cf. [14]]. 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. The latter can be achieved with the same or with the opposite direction. Such a control of motion is not possible with other engines such as the ratchet systems. 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 the driving frequency ω through $v = b\omega$, so that the maximum velocity is approximately given by $v_{\max} \approx (\pi/25)\sqrt{\Phi/m}$. For higher driving frequencies the motion gets first irregular and finally diffusive, losing its directionality. The wave vector q determines the correlation between the different rest lengths. A choice of $q = 1/5b$ turns out to yield a large maximum velocity and a "powerful" engine for $N = 3$. A measure for how powerful this engine is, is determined by a simple procedure [15], where the chain moves against a constant force applied at each particle. The chain with the parameters shown in Fig. 1 is able to move against a constant force of up to $F_{\max} \approx \Phi_0/b$, maintaining the velocity $b\omega$. For higher forces, the chain first remains in its initial location, and finally moves with the force. It is important to note that the maximum possible force depends sensitively on the parameters, in particular, on the constant c and the wave vector q. Another possible 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 interparticle 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.

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 it can easily be applied to other types of motion and generalized to higher dimensionality. Let us first discuss the case of higher dimensionality, and 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 $\Phi(x)$ by a 2D counterpart $\Phi(\vec{x}) = -\Phi_0\cos[\pi(\vec{x}^{(1)} - \vec{x}^{(2)})/b]\cos[\pi(\vec{x}^{(1)} + \vec{x}^{(2)})/b]$ ($\vec{x}^{(i)}$ denotes the ith component of the vector $\vec{x}$), and (d) the 1D interparticle potential $\Psi(x_i - x_{i+\delta_i})$ by the 2D counterpart $\Psi(\vec{x}_i - \vec{x}_{i+\delta_i}) = (k/2)[|\vec{x}_i - \vec{x}_{i+\delta_i}| - a_{i,i+\delta_i}(t)]^2$ [$|\cdot|$ denotes vector length]. Using the same form for $a_{i,i+\delta_i}(t)$ as in the case of 1D, the chain can be moved along the 2D surface. This raises the striking possibility of building a complex atomic scale "car" by connecting, for example, six chains in such a way that they constitute an array of 3×3 particles with 12 bonds; see Fig. 2(a) for a sketch of the geometry. By exciting three parallel chains coherently, this car can be moved both forward and backward as well as left and right [using the six vertical or the six horizontal bonds in Fig. 2(a)], so that it can be driven *freely* over the surface. As an example, shown in Fig. 2(b) are ten snapshots of the motion for a complete step of length

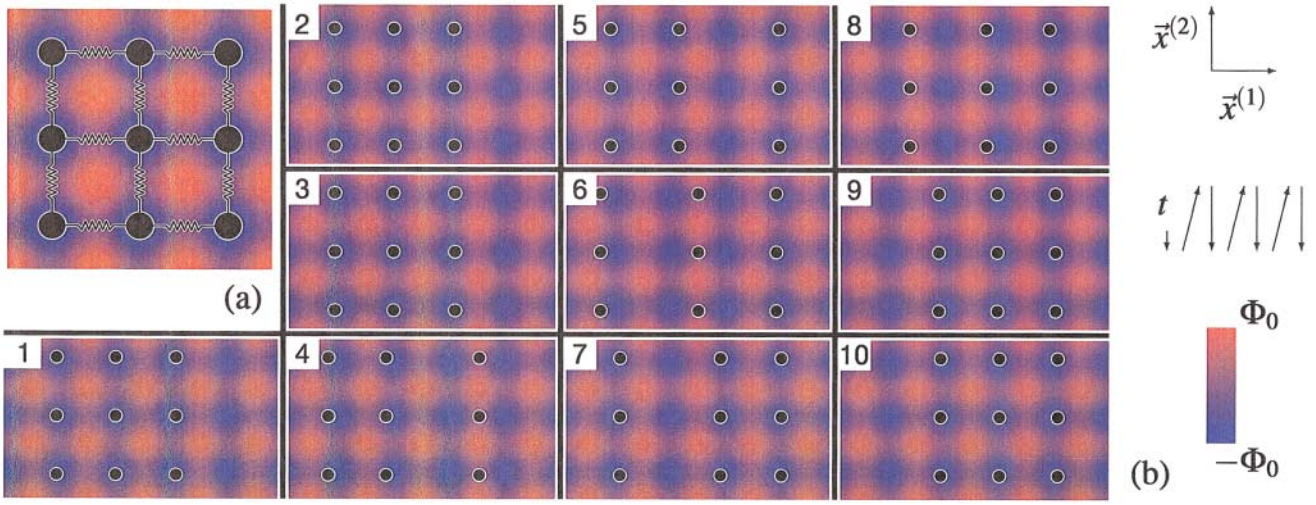

FIG. 2 (color). (a) Sketch of the 2D atomic scale "car" built by six chains arranged in an array of 3×3 particles. The surface potential $\Phi(\vec{x})$ is shown using the color code at the right. (b) Motion of the 2D atomic scale car sketched in (a); the black disks indicate the particles' position in relation to the surface potential in the ten numbered snapshots in time intervals of $(5b/2\pi)\sqrt{m/\Phi_0}$. The time $(25b/x)\sqrt{m/\Phi_0}$ of a full oscillation of the respective $a_{i,i+\delta_i}(t)$ and hence of a single step of length b to the right is shown. The parameters are identical to those in Fig. 1.

b to the right (note that the 10th snapshot is equivalent to the 1st as the car moved by a length b to the right).

Concerning the application to 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; see Fig. 3(a) for a sketch of a ring of $N = 3$ particles and $\ell = 4b$. This "wheel" can rotate either clockwise or counterclockwise. As an example, shown in Fig. 3(b) are ten snapshots of the rotation for a complete step of length b counterclockwise (note that the 10th snapshot is equivalent to the 1st as the wheel is rotated by a length b counterclockwise; for the fourfold symmetry of the example, this is equivalent to a rotation with an angle $\pi/2$ counterclockwise).

To demonstrate the robustness of our example engines and the concept in general, we should stress a few important points. First, it is clear that the motion of the chain is not affected by the integer part of the free rest lengths $a_{i,i+\delta_i}(t)/b$ between the particles or "feet" that touch the surface. In the above examples in Figs. 1 and 2, we have chosen the rest lengths $a_{i,i+\delta_i}(t)$ to oscillate between $11b/10$ and $187b/100$ (a relative change

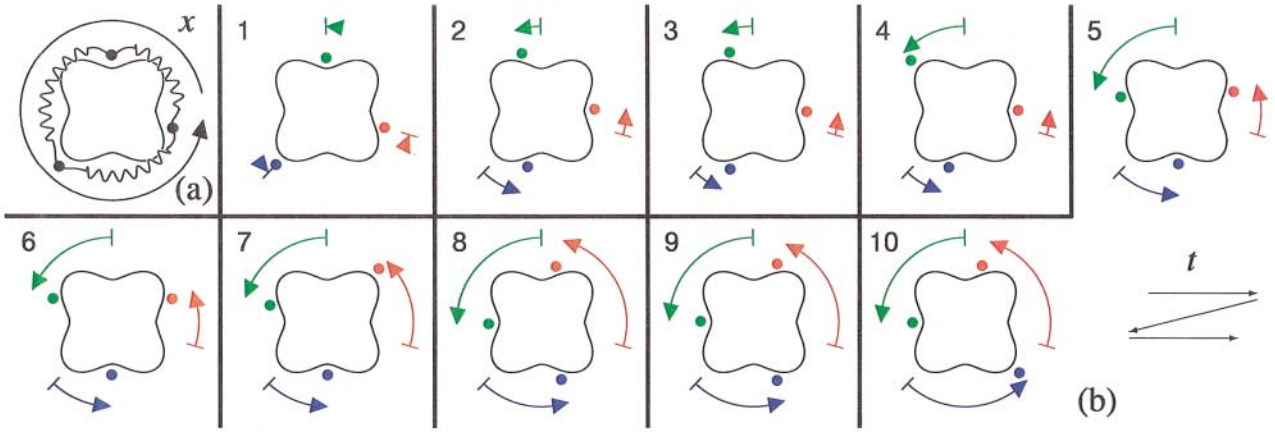

FIG. 3 (color). (a) Sketch of the atomic scale "wheel," showing the angular surface potential $\Phi(x)$ and the ring of $N = 3$ particles on a circle of circumference of length $\ell = 4b$. (b) Motion of the atomic scale wheel. The colored disks indicate the particles' position in relation to the angular surface potential in the ten numbered snapshots in time intervals of $(5b/2\pi)\sqrt{m/\Phi_0}$, where the arrows indicate the displacement relative to the first snapshot. The time $(25b/\pi)\sqrt{m/\Phi_0}$ of a full oscillation of $a_{i,i+\delta_i}(t)$ and hence of a rotational step of length b counterclockwise is shown (for the fourfold symmetry of the example this is equivalent to an angle $\pi/2$). Except $q = 1/3$ and $c = 3/10$, the parameters are identical to those in Figs. 1 and 2.

by $187/110$), but the same motion occurs for $a_{i,i+\delta_i}(t)$ oscillating between $21b/10$ and $287b/100$ (a relative change by $287/210$), between $31b/10$ and $387b/10$ (a relative change by $387/310$), and so on. Hence, the relative change can be made arbitrarily small. A second possibility to reduce the required stretching of the bond needed to cause a directed motion is to divide the $N-1$ bonds into g groups (N bonds in the case of rotational motion), each containing $(N-1)/g$ bonds (N/g bonds in the case of rotational motion), by setting $x_{i,i+1} = \mathrm{int}(i/g)b$ [$\mathrm{int}(x)$ denotes the largest integer n with $n \le x$]. For instance, for the parameters used for Figs. 1 and 2, but with $N = 10$ particles (i.e., 9 bonds) and $g = 3$ groups, each containing 3 bonds, it is sufficient that the free rest lengths $a_{i,i+\delta_i}(t)$ oscillate between b and $142b/100$ (instead of $11b/10$ and $187b/100$) to cause a directed translational motion with the same velocity $b\omega$.

One important question is that of the influence of the shape of the "excitation" $\alpha(s)$, which is sinusoidal in our case. As long as the excitation is approximately trapezoidal, a proper choice of driving frequency ω and wave vector q results in a directed motion. Since Eq. (1) is deterministic, another important question is that of the influence of noise. As long as the thermal energy $k_B T$ 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 $k_B T \gg \Phi_0$, the motion loses completely its directionality and becomes diffusive.

In comparison with other existing approaches to translational atomic scale engines, e.g., the ratchet systems mentioned earlier, or other models that use a spring with a time dependent length in combination with static/dynamic friction [16] or with a spatial asymmetric potential [17], the current approach has a number of advantages. In particular, our atomic scale engines can operate as microscopic "shuttles" or "trucks" that transport a cargo, a property that is absent in all other proposed schemes. In addition, the engines proposed here are not bound to a one-dimensional track and can be applied to different geometries and higher dimensionality.

As a conclusion, we would like to emphasize that the choice of a chain on a surface as the example engine has been motivated solely by the simplicity of the model rather than by experimental requirements. One important feature of the concept introduced here is that it does not impose any specific length or time scale. 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 here and might be applicable in a wide range of situations. A possible realization on an atomic or mesoscopic scale is by building 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 model, can be provided by individually controlling the bonds by light induced conformational changes of the chromophores. Using different chromophores which respond to different wavelengths should allow one to specifically excite bonds at chosen locations at given times. In this proposed realization the surface corrugation can be prepared by nanolithography. We believe therefore 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 breakthrough in the field of nanotechnology in providing new ways to manipulate molecules and clusters.

Financial support from the Israel Science Foundation, the German Israeli Foundation, and DIP and SISITOMAS grants is gratefully acknowledged. M. P. gratefully acknowledges the Alexander von Humboldt Foundation (Feodor Lynen program) for financial support.

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