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Molecular motor based entirely on the Coulomb interaction

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A molecular motor is introduced which is composed of charges only and which does not contain any potential or interaction besides the Coulomb one. The motor is shown to transform efficiently a driven random rotation into a directed translational motion. The direction of translational motion can be chosen dynamically, so that a ''forward gear,'' a ''reverse gear,'' and even a ''neutral gear'' exist. The high efficiency stems from the fact that this motor only steps in the direction determined by the chosen gear.

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Since almost 20 years ago the window to the ''nanometer-size world'' has been opened with the invention of scanning-tunnelling [1] and atomic force microscopies [2], these techniques have radically changed the way we view and interact with nanoscale objects making possible their imaging [3,4] and, even more important, their manipulation [4–8]. Although these achievements partly realize Feynman's visionary predictions [9], the important problem of further ''taming'' nanoscale objects and making them perform useful functions such as transportation still remains to be solved. Concerning these questions, one might on one hand learn from biological motors [10–14], or on the other hand make use of ''man-made'' concepts such as the one of competing lengths in a nonlinear system [15]. In fact, the stimulating interplay between biology and physics has been in part the motivation to investigate so-called ratchet systems, both theoretically [16] as well as experimentally [17]. Questions related to ratchet systems, however, had been studied already long ago in the rather general context of symmetry by Curie [18] and in the early days of the theory of Brownian motion [19], and are strongly related to the foundations of thermodynamics [20]. An important current issue is to bridge the gap between rather ''abstract'' ratchet-type potentials and possible simple physical realizations of man-made motors on molecular scale, which is still at its beginning.

In this Rapid Communication a man-made molecular motor is introduced which is composed of charges only and which does not contain any potential or interaction besides the Coulomb one, as for example the ratchet-type potentials mentioned above. The motor is constituted by two parts, the track and the moving entity. The track consists of a periodic but spatially asymmetric chain of alternating charges q and $-q$. The moving entity is a composite particle containing an arrangement of four charges, two charges q' and two charges $-q'$, having no net charge. It is shown that a rotation of the charge arrangement around its center of charge in one direction leads to a directed translational motion of the particle, whereas a rotation in the opposite direction leaves the particle localized at its original location. Thus, the motor shows a ratchet behavior similar to the one established recently [21]. Here, the open and blocked directions of translational motion are determined by the spatial arrangement of the particle's four charges. The motor is shown to perform an efficient directed translational motion even if the charge arrangement rotates in a random manner. By rearranging the particle's charges, in fact equivalent to a charge inversion, the open and blocked directions can be exchanged. As a result, the direction of motion can be chosen *dynamically* and a ''forward gear'' and a ''reverse gear'' exist. Additionally, there exists a charge arrangement where *both* directions of translational motion are blocked, corresponding to a ''no-load'' or ''neutral gear.'' The high efficiency stems from the fact that this motor only steps in the direction determined and allowed by the chosen gear.

The geometry of the proposed engine is sketched in Fig. 1: The track consists of charges $q>0$ at $\mathbf{t}_n^{(+)} \equiv \{(0.1+n)b,0,-0.25b\}$ and charges $-q$ at $\mathbf{t}_n^{(-)} \equiv \{(0.4+n)b,0,-0.25b\}$ with n integer, such that the track is charge neutral and periodic with periodicity b, but spatially asymmetric [see Fig. 1(a); the curly brackets $\{x,y,z\}$ denote a vector with components x, y, and z]. The moving entity is a composite particle with mass m at the center of mass coordinate $\mathbf{x}(x) \equiv \{x,0,0\}$ above the track. The particle contains in total four charges, namely, two charges $q_{11}=q_{12}=q'>0$ and two charges $q_{21}=q_{22}=-q'$, hence being charge neutral also [see Figs. 1(b) and 1(c)]. The four charges $q_{\mu\nu}=(-1)^{\mu}q'$ with $\mu,\nu=1,2$ rotate around the center of mass $\mathbf{x}(x)$ at po-

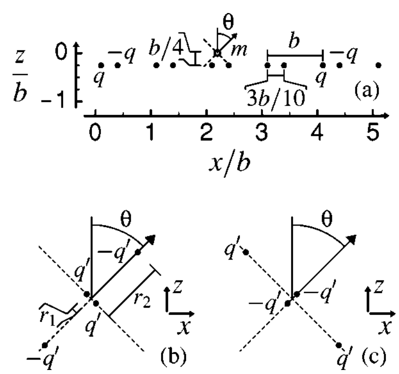

FIG. 1. Sketch of the engine geometry. In (a) the geometry of the track consisting of charges q at $\{(0.1+n)b,0,-0.25b\}$ and of charges $-q$ at $\{(0.4+n)b,0,-0.25b\}$ with n integer (closed circles) is shown. The particle with mass m, having the internal degree of freedom θ, is sketched as an open circle. In (b) and (c) the internal geometry of the particle consisting of two charges q' and of two charges $-q'$ (closed circles) is shown in detail for angle $\theta=\pi/4$, in (b) for $\gamma=1$ (''forward gear,'' corresponding to $r_1=0.005b$ and $r_2=0.05b$) and in (c) for $\gamma=-1$ (''reverse gear,'' corresponding to $r_1=0.05b$ and $r_2=0.005b$).

sitions $\mathbf{x}_{\mu\nu}(x,\theta)\equiv\mathbf{x}(x)+r_\mu\ \{\sin(\theta+\Delta\theta_{\mu\nu}),0,\cos(\theta+\Delta\theta_{\mu\nu})\}$ with phases $\Delta\theta_{\mu\nu}\equiv(\nu-\mu/2)\ \pi$. The two radii are given by $r_1\equiv[0.005+0.045\max(-\gamma,0)]b$ and $r_2\equiv[0.005+0.045\max(\gamma,0)]b$ (please note the different sign in front of γ), so that $0.005b\leqslant r_\mu\leqslant 0.05b$, and the center of mass is identical to the center of charge [22]. The parameter γ with $-1\leqslant\gamma\leqslant 1$ determines the "gear" of the motor. In Fig. 1(b) the arrangement of the particle's charges are shown for "forward gear" $\gamma=1$, and in Fig. 1(c) for "reverse gear" $\gamma=-1$. (The arrangement for 'neutral gear' $\gamma=0$ with $r_1=r_2=0.005b$ is not shown.) For all values of γ with $-1\leqslant\gamma\leqslant 1$ the four charges have a vanishing mono- and dipole moment, whereas the quadrupole moment depends on γ. Please note that $\gamma\rightarrow-\gamma$ together with $\theta\rightarrow\theta+\pi/2$ is equivalent to a charge inversion $q'\rightarrow-q'$.

The equation of motion of coordinate x reads as

$$m\ddot{x}+\eta\dot{x}+\frac{\partial\Phi(x,\theta)}{\partial x}=0, \tag{1}$$

where the damping is denoted by η. Since energy will be pumped into the system later on by varying the angle θ of the charge arrangement (see below), it should be emphasized that this energy has to be dissipated and hence $\eta>0$. Otherwise, the particle will gain energy until it decouples from the potential. The potential $\Phi(x,\theta)$,

$$\Phi(x,\theta)\equiv\frac{qq'}{4\pi\epsilon_0}\sum_{\mu,\nu=1}^{2}(-1)^{1+\mu}\sum_{n=-\infty}^{\infty}\left[\frac{1}{|\mathbf{t}_n^{(+)}-\mathbf{x}_{\mu\nu}(x,\theta)|}-\frac{1}{|\mathbf{t}_n^{(-)}-\mathbf{x}_{\mu\nu}(x,\theta)|}\right], \tag{2}$$

denotes the potential due to Coulomb interaction. Equation (2) can be rewritten as

$$\Phi(x,\theta)=\frac{qq'}{4\pi\epsilon_0}\sum_{\mu,\nu=1}^{2}(-1)^{1+\mu}[\phi(\mathbf{t}_0^{(+)}-\mathbf{x}_{\mu\nu}(x,\theta))-\phi(\mathbf{t}_0^{(-)}-\mathbf{x}_{\mu\nu}(x,\theta))], \tag{3}$$

introducing the lattice sum $\phi(\mathbf{r})$,

$$\phi(\mathbf{r})\equiv\sum_{\mathbf{n}}\frac{1}{|\mathbf{r}+\mathbf{n}|}\quad\text{for}\quad\mathbf{r}\neq 0, \tag{4}$$

as sum over $\mathbf{n}=\{nb,0,0\}$ with n integer. The lattice sum $\phi(\mathbf{r})$ in Eq. (4) has to be calculated using an Ewald summation technique [23], the lengthly result for the current geometry with periodicity in one direction only can be found in [24] and will not be repeated here. To simplify the notation, one can define an energy scale Φ_0 as the energy of a single charge q' being directly above one of the charges q of the track, e.g., for $x=0.1$, $\Phi_0\equiv qq'(4\pi\epsilon_0)^{-1}[\phi(\{0,0,0.25b\})-\phi(\{0.3b,0,0.25b\})]$, so that $|\Phi(x,\theta)|/\Phi_0<1\ \forall x,\theta$ (cf. Fig. 4 below).

Shown in Fig. 2 are the time evolutions of the particle translational coordinate x for all six combinations of the three values of gear $\gamma=1$, 0, and -1 and the two possibilities for the direction of rotation $\dot{\theta}<0$ and $\dot{\theta}>0$. As can be seen in the figure, there exist open and blocked directions for the translational motion of the particle, depending on the value of γ. For $\gamma=1$ [Figs. 2(a), and 2(b)], the forward direction is open and the backward direction is blocked, whereas for $\gamma=-1$ [Figs. 2(e) and 2(f)], the backward direction is open and the forward direction is blocked. For $\gamma=0$ [Figs. 2(c) and 2(d)], *both* the forward and the backward directions are symmetrically blocked, so that the particle remains localized in the vicinity of its starting point regardless of the direction of rotation $\dot{\theta}<0$ and $\dot{\theta}>0$. It is worthwhile to note that the inversion of open and blocked directions can also be achieved by a charge inversion of the track (i.e., $q\rightarrow-q$), but the neutral gear with both directions blocked cannot be realized by modifying the track. Even a rearrangement of the track's charges do not lead to the desired result. The only symmetrical situation for the particle motion that is achievable by moving the track's charges is that of a spatially symmetric charge arrangement, where, however, both directions are open and not blocked.

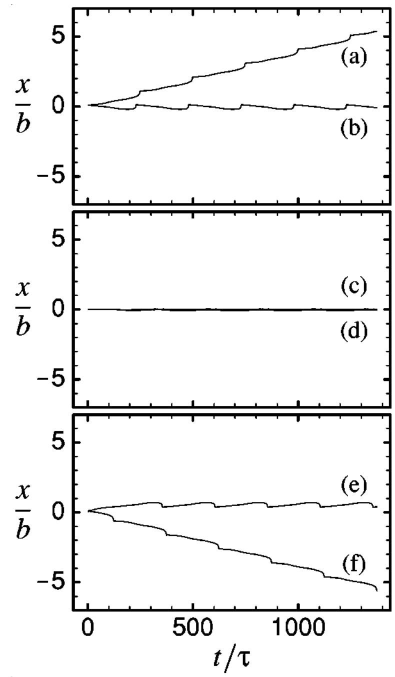

FIG. 2. Plot of the particle position x vs time t for three different values of the gear γ: (a) and (b) $\gamma=1$ ("forward gear"), (c) and (d) $\gamma=0$ ("neutral gear"), and (e) and (f) $\gamma=-1$ ("reverse gear"), for initial conditions $x=0$, $\dot{x}=0$, and $\theta=0$ at $t=0$. The absolute value of rotational velocity of the respective charge arrangement, $|\dot{\theta}|/[2\pi/\tau]=2\times10^{-3}$ with $\tau\equiv[(2\pi/b)\sqrt{\Phi_0/m}]^{-1}$, is identical in all six cases, with (a), (c), and (e) $\dot{\theta}>0$ and (b), (d), and (f) $\dot{\theta}<0$. The remaining parameter is the damping $\eta/[(2\pi/b)\sqrt{m\Phi_0}]=1$.

A simple modification of the constant rotational velocity presented in Fig. 2 is that of a rotational oscillation, e.g., of harmonic form $\theta=\theta_0+\theta_1\sin(2\pi\omega t)$ with an amplitude θ_1 and a frequency ω. For large enough amplitude ($\theta_1\gtrsim\pi/2$), the particle will perform a deterministic translational motion

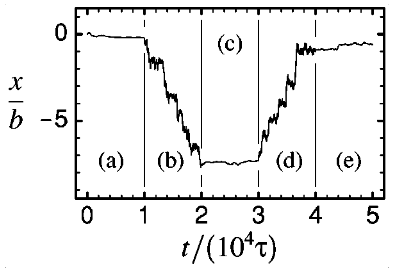

FIG. 3. Plot of the particle position x vs time t for a randomly rotating charge arrangement, for initial conditions $x=0$, $\dot{x}=0$, and $\theta=0$ at $t=0$. The absolute value of the rotational velocity $|\dot{\theta}|/[2\pi/\tau]=2\times 10^{-2}$ with $\tau\equiv[(2\pi/b)\sqrt{\Phi_0/m}]^{-1}$ is kept constant, and the direction of rotational velocity is randomly chosen anew every $\Delta t/\tau=1$. The values of the gear γ are (a) $\gamma=0$ (''neutral gear''), (b) $\gamma=-1$ (''reverse gear''), (c) $\gamma=0$ (''neutral gear''), (d) $\gamma=1$ (''forward gear''), and (e) $\gamma=0$ (''neutral gear''). The change of the charge arrangement caused by changing γ is performed continously within $\Delta t'/\tau=10$. The remaining parameter is the damping $\eta/[(2\pi/b)\ \sqrt{m\Phi_0}]=1$.

that is completely determined by the chosen gear γ. For ''forward gear'' $\gamma=1$, one observes an average velocity $\overline{\dot{x}}>0$ [25], for ''reverse gear'' $\gamma=-1$ one finds $\overline{\dot{x}}<0$ [25], and for ''neutral gear'' $\gamma=0$ the particle remains localized and $\overline{\dot{x}}=0$. The absolute value of average velocity $|\overline{\dot{x}}|$ depends on the choice of θ_0, θ_1, and ω [25]. For example, for $\theta_0=0$ and $\theta_1=\pi$ (for not too small damping $\eta \gtrsim (2\pi/b)\ \sqrt{m\Phi_0}$ and not too large frequency $\omega \lesssim [(2\pi/b)\sqrt{\Phi_0/m}]^{-1}$), one finds $|\overline{\dot{x}}|=2b\omega$.

A second possible and interesting scenario besides the constant rotational velocity or rotational oscillation cases is the one in which the angle θ performs a driven random motion; see Fig. 3. In the example shown, the angle θ performs the same type of driven random motion for the whole time shown in the figure. The gear, however, is changed from $\gamma=0$ [Fig. 3(a)] to -1 [Fig. 3(b)], then to 0 [Fig. 3(c)], afterwards to 1 [Fig. 3(d)], and finally back to 0 [Fig. 3(e)]. As can be seen in the figure, the particle remains localized for $\gamma=0$ [Fig. 3(a)], moves translational backward as the gear is changed to ''reverse'' $\gamma=-1$ [Fig. 3(b)], remains localized again at the new position for ''neutral gear'' $\gamma=0$ [Fig. 3(c)], moves forward as the gear is changed to ''forward'' $\gamma=1$ [Fig. 3(d)], and finally stays at the new position for $\gamma=0$ [Fig. 3(e)]. As a result, despite the permanent and random character of the driving, a detailed control of the particle motion is possible by a local rearrangement of the particle's charges. However, due to the random character of the driving, the translational motion of the particle is nevertheless stochastic in the sense that there exists an *average* velocity only. It is important to note that the random driving is *not* of thermal nature, but supplies energy to the system which is converted to directed transport. Hence, the reported behavior is (of course) not a violation of the second law of thermodynamics. The reason for studying this particular type of driving is that it represents the worst case of changing the angle θ: One only knows that θ (randomly) changes, but has no control over the actual value of θ.

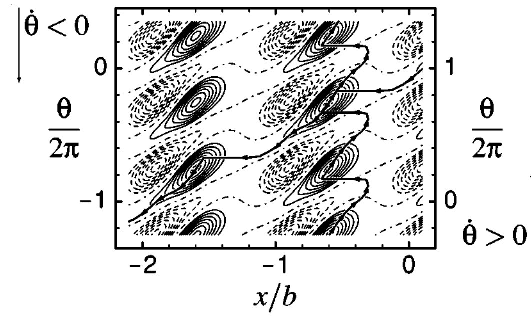

FIG. 4. Contour plot of the total potential $\Phi(x,\theta)$ due to Coulomb interaction for $\gamma=-1$. The equipotential lines are placed at $\Phi(x,\theta)=n\Phi_0/10$ with $-7\leqslant n\leqslant 7$ integer, and are solid for $\Phi(x,\theta)<0$, dashed for $\Phi(x,\theta)>0$, and dashed-dotted for $\Phi(x,\theta)=0$. The respective trajectories of a particle are shown for both $\dot{\theta}<0$ (left axis) and $\dot{\theta}>0$ (right axis) with thick lines, using $\eta/[(2\pi/b)\ \sqrt{m\Phi_0}]=10$ and $|\dot{\theta}|/[2\pi/\tau]=10^{-5}$ with $\tau\equiv[(2\pi/b)\sqrt{\Phi_0/m}]^{-1}$. The arrows indicate the time development for $\dot{\theta}<0$ (downward arrows) and $\dot{\theta}>0$ (upward arrows) and are placed every $\Delta t/\tau=10^4$.

To shed some light on the underlying dynamics of the observed behavior and to understand why and how the proposed mechanism works, it is helpful to look on the total potential $\Phi(x,\theta)$ due to Coulomb interaction, both as a function of x and θ. Shown in Fig. 4 is an example for $\gamma=-1$. Additionally to the potential, the respective trajectories of a particle are included for both $\dot{\theta}<0$ and $\dot{\theta}>0$. One observes that the particle mainly follows the time evolution of the local minimum in which it is located. There are, however, points of instability in the particle trajectories. In these points, the local minimum in which the particle has been located ceases to exist, and the particle follows the potential slope with respect to the coordinate x to the next minimum. In one case (rotation in the open direction), the further time evolution of the new minimum increases the distance gained by the jump, whereas in the other case (rotation in the blocked direction), the gained distance is canceled by the further time evolution of the new minimum. Both effects together result in the observed ratchet behavior. This behavior is strikingly similar to the ratchet behavior established in Ref. [21], although in the current system the total potential cannot be decomposed into two constant potentials which are translated with respect to each other as in Ref. [21]. Hence, it seems that the ratchet mechanism established in Ref. [21], despite the particular realization studied therein, is more general and of broader applicability. As the engine proposed here is quite robust in the sense that it is entirely based on the fundamental Coulomb interaction and that a *random* driving is sufficient, the described molecular motor should be feasible in actual experiments using already existing techniques, providing new ways to manipulate molecules and nanosize objects.

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