Molecular Motor with a Build-In Escapement Device

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Abstract. – We study dynamics of a classical particle in a one-dimensional potential, which is composed of two periodic components, that are time-independent, have equal amplitudes and periodicities. One of them is externally driven by a random force and thus performs a diffusive-type motion with respect to the other. We demonstrate that here, under certain conditions, the particle may move unidirectionally with a constant velocity, despite the fact that the random force averages out to zero. We show that the physical mechanism underlying such a phenomenon resembles the work of an escapement-type device in watches; upon reaching certain level, random fluctuations exercise a locking function creating the points of irreversibility in particle’s trajectories such that the particle gets uncompensated displacements. Repeated (randomly) in each cycle, this process ultimately results in a random ballistic-type motion. In the overdamped limit, we work out simple analytical estimates for the particle’s terminal velocity. Our analytical results are in a very good agreement with the Monte Carlo data.

Introduction. – A long standing challenge has been a problem of how to rectify unbiased random or periodic fluctuations into directional motion. For microscopic fluctuations, induced, e.g., by Brownian noise, this question has been debated since the inception of the random walk theory, and several important concepts have been worked out [1,2] (see also Ref. [3]). Indeed, it has been established already by Curie [4] more than a hundred years ago that although a violation of the $x \rightarrow -x$ symmetry is not sufficient to cause a net directional transport of a particle subject to a spatially asymmetric but on large scale homogeneous potential, the additional breaking of time reversal $t \rightarrow -t$ symmetry, (e.g., due to dissipative processes), may lead to a macroscopic net velocity, such that here directed motion can result in the absence of any external net force. These systems, known currently as thermal ratchets [5], have been subject of intensive research, both theoretical (see, e.g. Refs. [5,6,7,8,9,10,11,12,13,14,15,16]) and experimental (see, e.g. Refs. [17,18,19,20]). Advancements in this field have been summarized in Refs. [21,22,23].

On the macroscopic scale, the same problem of obtaining a useful work from random or periodic perturbations has been known for many centuries and this task has been indeed...
accomplished in many instances; to name but a few, we mention water- or windmills, or watches. In the latter case, the watch makers had to create a mechanism capable to convert the raw power of the driving force into regular and uniform impulses, which was realized by inventing various so-called escapement devices (see, e.g., Ref. [24]). Such a devise is most often a sort of a shaft or an arm carrying two tongues - pallets, which alternately engage with the teeth of a crown-wheel. The pallets follow the oscillating motion of the controller - the balance-wheel or a pendulum, and in each cycle of the controller the crown-wheel turns freely only when both pallets are out of contact with it. Upon contacts, the pallets provide impulses to the crown-wheel, (which is necessary to keep the controller from drifting to a halt), and moreover, perform a locking function stopping the train of wheels until the swing of the controller brings round the next period of release.

In this Letter we exploite the concept of such an escapement device to build a molecular motor capable of doing a ”useful work” under the action of random forces which average out to zero. The system we consider consists of a classical particle in a one-dimensional (1D) two-wave potential, which is is composed of two periodic in space, idencic time-independent components. One of them is externally driven by a random force and thus performs a random translational motion with respect to the other. This model has been previously proposed in Ref. [14] and it has been discovered that under certain conditions and for constant or periodic in time external driving force, the particle may perform totally directed motion with a constant velocity. Here we demonstrate that in such a system the particle may move unidirectionally with a constant velocity even in situations when the direction of the driving force (the controller) fluctuates randomly in time. We show that the physical mechanism underlying such a phenomenon is indeed that of an escapement-type device - upon reaching certain levels, random fluctuations exercise a locking function creating the points of irreversibility in particle’s trajectories such that, (despite the fact that the fluctuations average to zero), the particle gets uncompensated displacements. Repeated (randomly) in each cycle, this process ultimately results in a ballistic-type motion. Focussing on the overdamped limit, we use this physical picture to map the original system onto a Brownian motion (BM) process on a hierarchy of disconnected intervals. This allows us to work out simple analytical estimates for the particle’s terminal velocity, which are in a very good agreement with Monte Carlo data.

The Model. – Following Ref. [14], we consider a simple piece-wise continuous potential

\[
\Pi(x) \equiv \Pi_0 \begin{cases} 
-1 + \frac{2x}{\xi} & \text{if } x \leq \xi \\
1 - \frac{2x - \xi}{1 - \xi} & \text{if } x > \xi
\end{cases}, \quad (1)
\]

where the parameter \( \xi \in (0,1) \) determines the asymmetry of the potential, with \( \xi = 1/2 \) corresponding to the symmetric case. We will constrain our analysis here to the case \( \xi < 1/2 \). Note that it has a periodicity \( b = 1 \), so that \( \Pi(x + 1) = \Pi(x) \, \forall x \), an amplitude \( \Pi_0 = \max \Pi(x) = - \min \Pi(x) \), and one minimum is located at \( x = 0 \), i.e. \( \Pi(0) = -\Pi_0 \).

Now, the total potential \( V(x, \gamma) \) is the sum \( V(x, \gamma) \equiv \Pi(x) + \Pi(x - \gamma) \), where \( \gamma \) defines the external translation. Because of the periodicity of the potentials \( \Pi(x) \), the potential \( V(x, \gamma) \) is periodic in both arguments, so that \( V(x, \gamma + 1) = V(x, \gamma) \, \forall \gamma \). In this potential landscape, the equation of motion of a particle of mass \( m \) in a 1D medium with damping \( \eta \) reads:

\[
m\ddot{x}_t + \eta \dot{x}_t + \frac{\partial V(x_t, \gamma)}{\partial x_t} = 0, \quad (2)
\]
\( x_t \) being the particle’s trajectory. We note that energy is steadily pumped into the system through \( \gamma \), and is dissipated when \( \eta > 0 \), which prevents particle’s detachment.

Finally, we specify the properties of \( \gamma \). We suppose that \( \gamma \) obeys the Langevin equation, \( \dot{\gamma} = f_t \), where \( f_t \) is a random Gaussian, delta-correlated force with moments
\[
\overline{f_t} = f_0, \quad \overline{f_t f_{t'}} = f_0^2 + 2D\delta(t - t'),
\]
while the overbar denotes averaging over thermal histories. We will focus here mostly on the case \( f_0 = 0 \), such that \( \gamma \) is just a trajectory of a symmetric 1D BM. The case when \( f_0 \neq 0 \) or when \( \gamma \) represents anomalous diffusion will be briefly discussed at the end of the paper.

**Particles Dynamics in the Overdamped Limit.** We will restrict ourselves to the limit of an overdamped motion, \( \eta / \sqrt{m\Pi_0} \gg 1 \). As shown in Ref. [14], in this limit dynamics of the particle is governed entirely by the evolution of different minima of the total potential \( V(x, \gamma) \). Consequently, in order to obtain the trajectory \( x_t \) and the average velocity \( \overline{V} = \overline{x_t} \), it suffices to study the time evolution of positions of these minima. This process has been amply discussed in Ref. [14] and here we will merely outline the main conclusions.

According to Ref. [14], the particle’s dynamics proceeds as follows: the total potential \( V(x, \gamma) \) possesses a set of minima and position of each minima changes in time as the translation \( \gamma \) evolves. The particle, located at \( t = 0 \) at the first minimum simply follows the motion of this minimum up to a certain moment of time, or more precisely, a time moment when this minimum reaches a certain point \( x = \tilde{x} \). These \( \tilde{x} \)-points are the points of instability \( I \) in the \((x, \gamma)\) plane, where the corresponding local minimum of the potential \( V(x, \gamma) \) ceases to exist, and which emerge due to the asymmetry of \( \Pi(x) \). Further on, when the minimum disappears, a particle located at such a point performs an irreversible motion jumping to one of two neighboring minima, which still exist. Since the potential in the vicinity of each \( \tilde{x} \) may have both a downward and an upward bending, the jumps may be performed in both the leftward and the rightward directions. Depending whether \( \xi < 1/2 \) or \( \xi > 1/2 \), the leftward or rightward jumps may result in uncompensated or compensated displacements.

**Evolution of the effective translation.** We now put the particle’s dynamic rules deduced in Ref. [14] into a mathematical framework, amenable to analytical analysis, and introduce an auxiliary stochastic process \( \gamma_t \). We will call \( \gamma_t \) as an ”effective translation”, since it follows, apart of some special points (to be specified below), the evolution of the potential minima visited by the particle and keeps track of both the translation \( \gamma \) and the effect of the irreversibility points which induce particle’s leftward and rightward jumps to neighboring minima when the local minimum seizes to exist. We note also that the particle’s actual trajectory \( x_t = \gamma_t \) almost everywhere, except for some special points (to be specified below).

The effective translation \( \gamma_t \) obeys the following Smoluchowski-Feynman ratchet form:
\[
\dot{\gamma}_t = \hat{L}(\gamma_t) + f_t,
\]
where \( f_t \) are random forces defined in eq. 3, while \( \hat{L}(\gamma_t) \) is a local operator, which may be thought of as a space-derivative of some ”effective” potential.

This operator equals zero everywhere except for the set of special points \( \gamma_t = -K + \xi \) and \( \gamma_t = -K + 3/2, K = 1, 2, \ldots \). At these special points, the action of the operator \( \hat{L}(\gamma_t) \) is as follows: When \( \gamma_t \) reaches \( \gamma_t = -K + 3/2 \), (which we call the ”reflection point”), the operator \( \hat{L}(\gamma_t) \) changes \( \gamma_t \rightarrow \gamma_t - 1 \), (i.e. shifts its value from \( \gamma_t = -K + 3/2 \) to \( \gamma_t = -K + 1/2 \)). On the other hand, when \( \gamma_t \) hits \( \gamma_t = -K + \xi \), the operator \( \hat{L}(\gamma_t) \) shifts the position of the reflection point from \( -K + 3/2 \) to \( -K + 1/2 \), thus performing a ”locking” function - \( \gamma_t \) can not now return below the point \( -K + 3/2 \).
In Fig.1 we depict a typical realization of the process $\gamma_t$ for $f_0 = 0$. Note that because of $\hat{\mathcal{L}}(\gamma_t)$, $\gamma_t$ experiences an effective drift in the negative direction (for $\xi < 1/2$); for $\hat{\mathcal{L}}(\gamma_t) \equiv 0$ one should, of course, regain a standard result $\gamma_t \equiv 0$ and $\gamma_t^2 \equiv 2D_t$.

Note now that $\gamma_t$ can be viewed from a different perspective; namely, $\gamma_t$ can be regarded as a BM on a hierarchical lattice composed of a semi-infinite set of disconnected intervals of length $3/2 - \xi$ (see Fig.2). The process starts at $t = 0$ at the origin of the first interval ($K = 1$) and evolves freely until it either hits the right-hand-side (RHS) boundary $\gamma_t = 1/2$ (the reflection point), in which case it gets transferred instantaneously at position $\gamma_t = -1/2$ and continues its motion on the interval $K = 1$, or reaches the left-hand-side (LHS) boundary $\gamma_t = -1 + \xi$ - the "exit point" and gets irreversibly transferred to the second ($K = 2$) interval. In the second, and etc, interval $\gamma_t$ evolves according to the same rules.

The particle's trajectory $x_t$ follows the process $\gamma_t$, i.e. $x_t = \gamma_t$, except for two details: a) when $\gamma_t \in [-K + 1, -K + 3/2]$, $K = 1, 2, \ldots$, (thick lines in Fig.2), $x_t$ sticks to the left boundary of these intervals, such that the trajectories $x_t$ are saltatory with the random pausing times corresponding to the times spent by $\gamma_t$ in the intervals $[-K + 1, -K + 3/2]$, $K = 1, 2, \ldots$, (see Fig.1). b) the event when $\gamma_t$ hits the LHS boundary of the $K$-th interval and gets instantaneously transferred to the next interval (i.e. $\gamma_t$ does not have a discontinuity) corresponds to the event when the particle makes a jump from $x_t = -K + \xi$ to $x_t = -K$, i.e. at this point $x_t$ changes discontinuously. On the other hand, it is clear that such jumps do not contribute to the average particle velocity $\bar{x}_t$ and hence, $\bar{x}_t = V = \gamma_t$.

**Particle’s terminal velocity.** – We turn next to the computation $V$ for $f_0 = 0$. Evidently, even in this simplest case the map depicted in Fig.2 is too complex to be solved exactly. However, some simple analytical arguments can be proposed to obtain very accurate estimates...
of $V$. To do this, we first note that it is only when passing from the $K$-th interval to the $(K+1)$-th one, (which is displaced on a unit distance on the $\gamma_t$-axis with respect to the previous one), the process $\gamma_t$ gains an uncompensated (negative) displacement equal to the overlap distance of two consecutive intervals, i.e., $1/2 - \xi$. Consequently, we may estimate $V$ as

$$V = -\frac{1}{T} \left( \frac{1}{2} - \xi \right)$$

where $T$ is the mean time which $\gamma_t$ "spends" within a given interval.

To estimate $T$, let us consider how $\gamma_t$ evolves on a given interval; $T$ is, as a matter of fact, the mean time needed for $\gamma_t$ to reach diffusively for the first time the LHS boundary of the interval - the "exit" point $-K + \xi$, starting from the "entry" point $-K + 1 + \xi$ (see Fig.3). We divide next the $K$-th interval into three sub-intervals:

$$l_1 = l_2 = \frac{1}{2} - \xi \quad \text{and} \quad l_3 = 1/2 + \xi$$

Since $l_1 = l_3 \leq l_2$, for typical realizations of $f_t$, the following scenario should hold: $\gamma_t$ evolves randomly around the "entry" point and first hits the RHS boundary of the $K$-th interval passing thus through the sub-interval $l_1$; the mean time required for the first passage of $l_1$ is denoted as $T_1$. For BM with diffusion coefficient $D$, $T_1 = (1/2 - \xi)^2 / 2D$ [25]. Further on, after hitting the RHS boundary, $\gamma_t$ gets reflected to the point $\gamma_t = -(2K-1)/2$ and evolves randomly around this point until it hits the LHS boundary of the interval - the "exit" point. For symmetric BM, the time $T_3$ needed for the first passage through $l_3$ is equal to $T_1$. Consequently, $T = T_1 + T_3 = (1/2 - \xi)^2 / D$ and the velocity reads

$$V = -2D \left( 1 - 2\xi \right)^{-1}$$

In Fig.4 we compare our prediction in eq.(5) and the results of Monte Carlo simulations, which shows that theoretical arguments presented here capture the essential physics underlying the dynamics of the random map depicted in Fig.2 and, hence, of the process in eqs.(2) and (3).

Now, several comments on the result in eq.(5) are in order.

(i) First, we note that $V$, eq.(5), diverges when $\xi \to 1/2$ (note, however, that $V \equiv 0$ for $\xi \equiv 1/2$), which is a seemingly counter-intuitive behavior. Such a behavior stems, as a matter of fact, from our definition of $\gamma_t$: namely, by writing our eq.(4), we tacitly assume that both the effective step $\delta \gamma$ of the process $\gamma_t$ and the characteristic jump time $\tau$ are infinitesimal
variables, (while the ratio \( D = (\delta \gamma)^2/2\tau \) is supposed to be fixed and finite). On the other hand, for any real system \( \delta \gamma \) and \( \tau \) might be very small but nonetheless are both finite. For finite \( \delta \gamma \) and \( \tau, \gamma \) is a symmetric hopping process on a lattice with spacing \( \delta \gamma \) and with the characteristic time \( \tau \). Then, we have \( T_1 = T_3 = \tau (1 + L) L \), where \( L = (1/2 - \xi)/\delta \gamma \) is the number of elementary steps \( \delta \gamma \) in the interval \( (1/2 - \xi) \). This yields, in place of eq. (5),

\[
V = -2D (2\delta \gamma + 1 - 2\xi)^{-1},
\]

where now \( V \) tends to a finite value when \( \xi \to 1/2 \) (but still \( V \equiv 0 \) when \( \xi \equiv 1/2 \)).

(ii) Second, notice that \( V \) in eq. (5) is a monotonously increasing function of \( \xi \); that is, the absolute value of \( V \) is maximal when \( \xi \to 1/2 \) and minimal, \( |V| = 2D \), for the strongest asymmetry, \( \xi = 0 \). We note that such a behavior again stems from the definition of \( f_t \) as a Gaussian, delta-correlated noise. On the other hand, since \( f_t \) is influenced by some external processes, it might be characterized, e.g., by correlations or be a non-local in space or in time (discontinuous) stochastic process. In both cases, the behavior of \( V \) in the presence of such an external force would be different of that predicted by eqs. (5) and (6).

Consider now what will happen if \( f_t \) represents the so-called delta-correlated Lévy process (LP) with parameter \( \mu \) (see an exposition in excellent Ref. [25] for more details). We note here parenthetically that the case \( \mu = 2 \) corresponds to the usual Gaussian case, which yields conventional BM, while the case \( \mu = 1 \) describes the so-called Cauchy process.

Now, what basically changes when we assume that \( f_t \) is the LP, is the form of the first passage times \( T_1 \) and \( T_2 \). Here, the time required for the first passage of an interval of length \( 1/2 - \xi \) reads \( T_1 = T_3 = (1/2 - \xi)^{\mu} \) \[25\] and hence, \( V \sim -(1 - 2\xi)^{1-\mu} \).

Consequently, we infer that \( V \) will be a monotonously increasing function of the parameter \( \xi \) only for the LP with \( \mu > 1 \), i.e., for the persistent processes (which have a finite probability for return to the origin). In the borderline case of \( \mu = 1 \) velocity will be independent of the asymmetry parameter. On contrary, for transient (having zero probability of return to the origin) processes with \( \mu < 1 \), which are not space-filling (fractal) and occupy the space in clustered or localized patches, one would find that \( V \) is a decreasing function of \( \xi \).

(iii) Finally, we consider the case when the bias is oriented in the positive direction, i.e. \( f_0 \geq 0 \). In this case, \( \gamma_1 \) is an asymmetric hopping process on a 1D discrete lattice of spacing \( \delta \gamma \) and with transition probabilities \( p (q) \) of jumps in the positive (negative) directions which obey \( p/q = \exp(\beta f_0 \delta \gamma) \), with \( p + q = 1 \), where \( \beta \) denotes the reciprocal temperature.

Here, the symmetry \( T_1 = T_3 \), which exists for \( f_0 = 0 \), is broken: when passing through \( l_1 \) the process \( \gamma_t \) follows the field, while the passage through \( l_3 \) takes place against it. Supposing that \( \delta \gamma \) and \( \tau \) are both finite, we have that here:

\[
T_{1,3} = \frac{\tau}{p - q} \left[ \pm \frac{1 - 2\xi}{2\delta \gamma} + \frac{\phi_1}{p - q} \left( \frac{p}{q} \right)^{\tau/(1 - \xi)} - 1 \right],
\]

where the upper (lower) sign corresponds to index "1" ("3"), while \( \phi_1 = q \) and \( \phi_3 = p \). Note that \( T_1 \) grows linearly with the sub-interval length \( 1/2 - \xi \), while \( T_3 \) shows much stronger, exponential interval-length dependence, and hence, controls the overall time spent within a given interval. Consequently, the particle’s velocity in this case attains the form

\[
V = -\frac{(1/2 - \xi) \sinh^2 \left( \beta f_0 \delta \gamma/2 \right)}{\tau \cosh \left( \beta f_0 \delta \gamma/2 \right) \left[ \cosh \left( \beta f_0 (1 - 2\xi + \delta \gamma)/2 \right) - \cosh \left( \beta f_0 \delta \gamma/2 \right) \right]},
\]
which reduces in the diffusion limit to the following result

\[ V = -\frac{(1-2\xi)D\beta^2f_0^2}{8\sinh^2\left(\beta f_0(1-2\xi)/4\right)} \]  

(9)

The salient feature of these results is that here the particle’s drift proceeds against the applied field, due to fluctuations in the process \( \gamma_t \) - some (exponentially small) number of trajectories which travel against the field.

In conclusion, we have studied dynamics of a classical particle in a 1D potential, composed of two periodic components, one of which is driven by an external random force. We have shown that in such a system the particle may move unidirectionally with a constant velocity even when the random driving force averages out to zero. We have demonstrated that the physical mechanism underlying such a behavior resembles the work of the so-called escape-device, used by watch makers to convert the raw power of the driving force into uniform impulses; here, indeed, upon reaching certain levels, random forces lock the particle’s motion creating the points of irreversibility, such that the particle gets uncompensated displacements. Repeated (randomly) in each cycle, this process ultimately results in a ballistic-type motion. Concentrating on the overdamped limit, we have used this picture to map the original system onto a BM process on a hierarchy of disconnected intervals, which allowed us to present analytical estimates for the particle’s velocity. Our analytical results are in a very good agreement with Monte Carlo data. Extensions for systems with other than Gaussian fluctuations and systems with global bias have also been presented.

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