Transient dynamics in the thermal ratchets transport model

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The thermal ratchets model toggles a spatially periodic asymmetric potential to rectify random walks and achieve transport of diffusing particles. We numerically solve the governing equation for the full dynamics of an infinite 1D ratchet model in response to periodic switching. Transient aperiodic behavior is observed that converges asymptotically to the period of the switching. We study measures of the transport rate, the transient lifetime, and an equivalent of ‘amplitude’, then investigate their dependence on various properties of the system, along with other features of the transient and asymptotic dynamics.

I. INTRODUCTION

Pure diffusion is isotropic, not resulting in transport in any particular direction. A potential gradient induces drift in addition to the diffusion, and may result in transport. In overdamped environments, any external force induces a proportional drift velocity \( v = F/\gamma = -\frac{1}{\gamma}U_x \) (subscripts denote partial derivatives), where \( U \) is the potential energy. Thus, a potential whose space-averaged force is zero will not naively be expected to result in non-zero average transport. But the thermal ratchets model achieves this by rectifying diffusion [1, 2]. The most common form studied is a spatially periodic asymmetric sawtooth (‘ratchet’-shaped) potential (see Fig. 1), exerted over a 1D array of diffusive particles. The potential is switched on and off either periodically or stochastically, and results in the transport of diffusing particles in the direction of the gentler sawtooth slope.

Possible applications of the model are in approximating transport phenomena by molecular motors [3, 4], or to construct experimental or theoretical setups that achieve long-range transport of diffusing particles without requiring a long-range potential gradient. Several previous works have analyzed the model via either an analytical Fokker-Planck approach, Monte Carlo simulations, or experimental setups, and have investigated in particular the resulting particle flux and its dependence on various factors [5–10].

The governing equations for the particle concentration cannot be solved analytically for the full dynamics in general, only under certain assumptions (say spatio-temporal periodicity), or to yield the steady state. To study the full dynamics, we employ a finite difference numerical method, with the potential switched at equal ON and OFF periods. Our results show that the dynamics is initially aperiodic in time. With continuing switching cycles, it asymptotes to the period of the switching, during which the concentration oscillates between shapes we shall call ‘turning curves’. We shall study the dynamics of the particle concentration and investigate the transport rate for the transient and the asymptotic periodic behavior. We also investigate the dependence of these on various system parameters.

II. ANALYSIS

In an infinite 1D system of independent particles, the dynamics of their concentration is governed by the following Fokker-Planck equations which are the drift-diffusion equations:
Inconveniently, the flux $J$ evaluated at some arbitrary position does not represent the macroscopic transport of particles. Local fluxes may be countered by opposite fluxes at other positions and therefore are not a quantifier of the long-range transport. Spatially averaging $J$, however, serves to cancel out internal flows and yields only the global transport that is the goal of the system.

Now, since the dynamics maintains the spatial period of the potential, so does the flux. Averaging it over a single period $\lambda$ then serves as well as over all space, and we define the space-averaged flux, or transport rate as (see [2]):

$$ T(t) = \frac{1}{\lambda} \int J \, dx = \frac{1}{\lambda} \int (vc - Dc_x) \, dx. \quad (3) $$

Owing to the spatial periodicity of $c$, the second term integrates to zero, and we have:

$$ T(t) = \frac{1}{\lambda} \int vc \, dx = -\frac{1}{\gamma \lambda} \int cU_x \, dx. $$

Observe now that the transport will vanish whenever the concentration is a function of the potential, i.e., $c(x) = c(U(x))$, owing to the periodicity of $U$. Graphically, this is the case when the two pieces of the concentration over the shallow and steep ratchet slopes are mirrored and horizontally scaled versions of each other proportional to their slope widths. The drift speed on the other hand being inversely proportional to the slope widths and in opposite directions ensures the net zero integral. The steady state Boltzmann distribution $c(x)e^{-U(x)/\gamma D}$ is a special case of this situation.

Zero transport is thus a more general situation than steady state. Even out of equilibrium, there is no transport when $v = 0$, i.e., in absence of drift. This has the following physical interpretation. Pure diffusion from any initial concentration profile relaxes it to a flat one. The local fluxes $J$ of these equilibrating flows shall depend on the particular initial distribution, but their space-average is zero, i.e., they achieve no transport. One way to understand this is in the context of the Green’s function: recall that the particles are independent, hence diffusion from any distribution is a superposition of diffusion from point sources, each of which is a spreading symmetric Gaussian with zero space-averaged flux.

Thus, the transport rate defined derives only from drift and not from diffusion. Interestingly though, diffusion is indispensable for the mechanism in that in the OFF state it evolves the concentration distribution, which affects the above integral once the potential turns back on. More physically, diffusion is what is rectified by the spatial asymmetry to produce directed transport.

III. TRANSIENT DYNAMICS

Upon initiating pumping, the dynamics is aperiodic, but it asymptotically converges to the period of the

\[ J = vc - Dc_x \]  
\[ c_t = -J_x = Dc_{xx} - (vc)_x = Dc_{xx} + \frac{1}{\gamma}(cU_x)_x \]  
\[ \dot{\hat{c}}_t = \hat{D}\hat{c}_{\hat{x}\hat{x}} + (\hat{\hat{U}}_x)_{\hat{x}} \]

where $\hat{t} = t/\tau$ and $\hat{x} = x/\lambda$ measure time and space in multiples of the temporal and spatial ratchet periods, $\hat{c} = \lambda c$ is a dimensionless concentration density, $\hat{D} = D/D_0$ is a scaled diffusion coefficient, and $\hat{U} = U/E_0$ is a scaled potential energy. Defining the form of the asymmetric sawtooth potential requires specifying the degree of skewness of the ratchet shape $\alpha = a/\lambda$, and the scaled amplitude $\hat{U}_{max} = U_{max}/E_0$ (see Fig. 1). These and $\hat{D}$ constitute the three dimensionless parameters that govern the character of our system. Results that follow shall be accompanied by the parameter values at which particular behavioral features are highlighted. However, we shall also discuss dependencies on dimensional parameters such as $D$ and $\tau$, as their variations are more practical to consider in a physical setup.

Solved analytically for the steady state, the particle density lies in a Boltzmann distribution in response to the potential profile. By Eq. (2), the steady state condition $c_t = 0$ enforces uniform flux over space. It may be shown that the flux in fact vanishes everywhere [11], unless there exists an additional external force, in which case there is a uniform flux in its direction. However, switching the potential at finite intervals prevents the attainment of the steady state, but achieves transport even in the absence of any further external force.

At this point we make the simplifying assumption of spatial periodicity with the following argument. Initializing with a concentration that has the spatial period of the potential, its ensuing dynamics shall also be periodic at all times, since all terms of Eq. (2) and boundary conditions stay identical in each spatial period. We thus start from a flat (trivially periodic) concentration and solve the equation on a single spatial period with periodic boundary conditions, reproducing the behavior expected on an infinite line.
switching. First we illustrate this behavior, and later provide a physical reasoning.

In Fig. 2 we plot the numerical time-integral of the transport rate $T(t)$, i.e., the cumulative number of particles transported over time. The cumulative local flux, i.e., the time-integral of $J(x,t)$, at two arbitrary positions, is plotted alongside for illustration. These integrals are reset to zero at the start of each ON phase, to aid comparison between cycles.

In accordance with the previous arguments, the cumulative transport curve is observed to be flat during the OFF phases, although the local fluxes vary smoothly over the entire cycle, and differently at different positions. Interestingly, the dynamics passes through an intermediate maximum of transport before attaining periodicity. The entire dynamics attains periodicity, which is why, for example, the curves of the two local fluxes also exhibit periodicity at the end. Also interesting is that in the final periodic dynamics, the transport at the start of each cycle is briefly backwards (negative) before it compensates and moves forward.

We seek a measure of convergence to periodicity. Call $J_{cyc}(x)$ the integral of $J(x,t)$ over an on-off cycle, i.e., the number of particles passing through a point over a cycle. As the dynamics converges to periodicity, one must expect this to converge to the same value at every position (equal to its spatial mean $T_{cyc}$, the transport integrated over a cycle). Otherwise there would be accumulations or depletions between different positions in each cycle, and they would grow unboundedly now that the dynamics is periodic, breaking particle conservation.

Thus the standard deviation of $J_{cyc}(x)$ over the spatial period provides such a measure. Dividing by the mean $T_{cyc}$ yields the spatial coefficient of variation, a more uniform measure that accounts for the variation of the asymptotic transport rate itself. We use this as the measure of approach to periodicity, and plot it against cycles on the secondary axis of Fig. 2. As expected, it is seen to decay asymptotically as the dynamics converges to periodicity.

If such a pumping system operates for a long time, the long-term transport rate shall be the asymptotic periodic one. Thus, in discussions of the transport rate of the model for a choice of parameters, the quantity of interest is the asymptotic rate, which as we noted is unfortunately lower than the intermediate maximum.

Now we attempt to explain the transient and long-time periodic behavior via the following mechanism. In each ON phase the drift pushes the concentration towards the potential valleys against a gradually mounting diffusive resistance. In the OFF phase the diffusion undoes some of this by spreading it back out. However, with continuing cycles, the drift succeeds in incrementally advancing this turning point, until the progress due to drift in the ON phase is exactly pushed back by the diffusion in the OFF phase. The concentration then settles into a periodic oscillation between the distributions at the turning points, which shall be discussed in further detail.
IV. TRANSIENT LIFETIME AND LONG-TERM TRANSPORT RATE

In light of the previous discussion, we first define the transient lifetime to be the number of cycles elapsed until the coefficient of variation of \( J_{\text{cyc}}(x) \) drops below 1%. We observed that both the transient lifetime, and the average asymptotic rate \( T_{\text{cyc}}/\tau \) that the transport converges to, depend on the diffusion coefficient \( D \) as well as the duration of the switching cycle \( \tau \). To study the latter, we use the ‘settling time’ as a time scale of the system against which to measure the switching period. This is defined as the maximum time required to equilibrate in the ON phase when we disregard diffusion. It is given by the time taken by a particle to traverse the gentler ratchet slope with the drift speed in that region, and is given by \( t_{\text{set}} = b^2 \gamma / U_{\text{max}} \).

In Fig. 3 (a) and (b) we plot the variation of the transient lifetime and the asymptotic average transport rate (normalized by the uniform starting concentration height) in response to varying either \( \tau \) or \( D \) while keeping the other fixed. In the dimensionless formulation, both amount to varying \( D \) proportionally. Therefore, in plots (a) - (c) of Fig. 3, the scales of the two horizontal axes have been adjusted so that any abscissa indicates the same value of \( D \) on either axis, which ranges from 0 to \( \approx 0.36 \) over the horizontal range of the plot. The two curves differ since varying \( \tau \) at fixed \( D \) also entails varying \( U_{\text{max}} \) proportionally (it ranges from 0 to \( \approx 146 \) over the \( \tau \)-axis), while upon varying \( D \) at fixed \( \tau \) it is unchanged (fixed at 30 over the \( D \)-axis). Yet, their trends are similar, due to the following reason.

The asymptotic transport rate exhibits a local maximum against both \( D \) and \( \tau \). At large \( D \) the concentration hardly responds to the potential, barely moving from the initial flat profile, impeding transport.

Transit lifetime drops with increasing period length and diffusivity. Increasing \( D \) at fixed \( \tau \) causes the incremental advance with continuing cycles due to drift to stop sooner, while increasing \( \tau \) at fixed \( D \) allows the drift more time to advance the concentration until it rests against diffusive pressure. Both lead to the attainment of the periodic oscillatory dynamics within fewer cycles.

The responses of the mean asymptotic transport rate and the transient lifetime to the degree of skewness of the ratchet have been illustrated in Fig. 4. The behavior of the transport rate is more readily understood. \( \alpha \in \frac{1}{2} \) corresponds to the right (left) slope being the gentler slope, causing transport in that direction. (We have plotted the absolute rate, i.e. positive in both directions.) The greater the skewness, the higher the rectification and therefore the transport rate. A symmetric ratchet shape naturally yields no transport.

The explanation behind the variation of the transient lifetime is more involved. As described previously, periodicity is attained when a balance is struck between the advance of the particles by drift and their retrograde dif-
fusion over each cycle. The relative strengths of the two
determine how many cycles elapse until this balance is
attained. High and low skewness tilt the balance strongly
in favour of the drift and diffusion respectively, both as-
sisting in quicker attainment of the final oscillatory equi-
lbrium. An intermediate skewness causes the concentra-
tion to both advance and roll back by a great extent in
each cycle, which takes longer to settle into an exactly
balanced rhythm.

V. ASYMPTOTIC PERIODIC OSCILLATION
BETWEEN TURNING CURVES

The steady state Boltzmann distribution consists of
two piecewise exponentials in the ON phase of the poten-
tial, and is flat for the OFF phase (dashed curves in
Fig. 1). Call these \( c_{\text{eq}}(x) \) and \( c_{\text{off}}(x) \) respectively. If the
concentration reaches steady state at the end of either
or both phases, the dynamics shall be identical in each
cycle. For example, if the concentration reaches equilib-
rium at the end of each ON phase, the diffusive dynamics
of the OFF phase shall begin from this steady state and
proceed identically in each cycle until it is interrupted at
the same point by the potential turning ON.

However, switching the potential with a finite period
prevents the concentration from reaching equilibrium in
either phase. In the asymptotic behavior, the dynam-
ics is nevertheless periodic, as the concentration on its
way to either of the equilibria is interrupted at the same
two points by the potential switching. The solid curves
in Fig. 1 represent these ‘turning point’ profiles at the
switchings, between which the concentration oscillates.
Call the turning curves at the end of the ON and OFF
phases as \( c_{\text{eq} \text{turn}}(x) \) and \( c_{\text{off} \text{turn}}(x) \) respectively.

Oscillation between the two steady states would al-
low the maximum possible ‘amplitude’, but is not possi-
ble with a finite switching period. The turning curves
represent the end points of a restricted, smaller am-
plitude oscillation. A natural quantity to study there-
fore is the departure of the turning curves from the
Corresponding steady state distributions, representing
the fraction of the maximum amplitude covered. To
quantify this, we measure the difference in shape be-
tween two curves by the \( L_1 \)-distance within a period:
\[
d_1(f, g) = \int |f(x) - g(x)| \, dx,
\]
In terms of the area contained between them (highlighted in Fig. 1). We consider
\[
d_1(c_{\text{eq} \text{turn}}) + d_1(c_{\text{off} \text{turn}})
\]
as a measure of departure of
the turning curves from the steady states. We normalize
this as a fraction of the distance between the two steady
states \( d_1(c_{\text{eq}}, c_{\text{off}}) \) and define:
\[
\delta = \frac{d_1(c_{\text{eq} \text{turn}}) + d_1(c_{\text{off} \text{turn}})}{d_1(c_{\text{eq}}, c_{\text{off}})}
\]

We plot \( \delta \) in Fig. 5 (a) against increasing switching
period (measured in units of \( t_{\text{set}} \)), and \( D \), each while
keeping the other constant as before.

Increasing the forcing period allows the concentration
more relaxation time to evolve towards steady state in
each phase, and the turning profiles should be closer to
the corresponding Boltzmann equilibrium profiles. Ac-
Accordingly, \( \delta \) was seen to decrease smoothly and monoton-
ically with increasing switching period and go asymptot-
ically to 0 for long periods. It is greatest in the limit of
zero switching period, when the concentration does not
move from its initial uniform distribution (which is also
\( c_{\text{eq}} \)), and the ratio is therefore 1.

The response to varying \( D \) is similar, but its explana-
tion is different. At the limit of vanishing \( D \), diffusion
barely rolls back the advance due to drift in each cy-
cle, and thus with continuing cycles the concentration
incrementally and asymptotically advances towards the
ON phase steady state \( c_{\text{eq} \text{on}} \), and is hardly pushed back
in the OFF phase. Therefore, in the asymptotic periodic
dynamics, the profiles \( c_{\text{on} \text{turn}} \) and \( c_{\text{off} \text{turn}} \) are both almost
the same as \( c_{\text{eq} \text{on}}, c_{\text{eq} \text{off}} \), however, is still the flat profile (at
\( D = 0 \), \( c_{\text{off}} \) would also be the same as \( c_{\text{eq} \text{off}} \), but recall that
we are instead considering \( D \to 0 \)). Therefore, both the
numerator and denominator of \( \delta \) become \( d_1(c_{\text{eq}}, c_{\text{off}}) \)
in this limit, yielding 1.

At high \( D \), \( c_{\text{eq}} \) is only slightly deviated from the flat
\( c_{\text{eq} \text{off}} \), yielding a small denominator. As noted before, the
approach towards the steady state \( c_{\text{eq} \text{on}} \) is faster at higher
\( D \), so that \( c_{\text{on} \text{turn}} \) is almost coincident with it. Also the
high diffusion rapidly rolls back this drift almost entirely in
every OFF stage, so that \( c_{\text{off} \text{turn}} \) is nearly coincident with \( c_{\text{off}} \). Thus, with rising \( D \), both terms in the numer-
ator drop more sharply than the denominator, yielding a
decaying \( \delta \).

As the skewness \( \alpha \) of the ratchet potential shape is
varied, \( \delta \) exhibits a maximum for a symmetric ratchet
shape, and a minimum for an intermediate skewness, but
the variation is overall weak compared to the response
against other parameters. This variation is related to

\[
\alpha = \frac{a}{\lambda}
\]
FIG. 5. Response of $\delta$, a measure of deviation of the turning curves from the steady state distributions, against some system parameters. (a) $\delta$ decays with increasing $D$ and $\tau$. Parameter values and axis scale adjustments same as Fig. 3. (b) $\delta$ exhibits a maximum for a symmetric ratchet potential shape and a minimum for an intermediate degree of skewness $\alpha$. However, the overall variation is small. Parameters same as Fig. 4.

details of how the shapes of the equilibrium and turning curves shift in response to changing skewness, and does not have a strong and immediate physical cause.

VI. CONCLUSIONS

We employed a numerical solution of the governing drift-diffusion equations of an infinite 1D thermal ratchets model to yield its full dynamics, and observed that initially aperiodic dynamics converges to the period of the switching. We defined measures of the large-scale transport achieved by the system and the transient lifetime. The transport rate maximizes at a finite diffusivity $D$ and switching period $\tau$, and increases with greater skewness of the asymmetric ratchet shape. The transient lasts for fewer switching cycles upon increasing $D$ or $\tau$, and lasts longest at an intermediate skewness.

The long-term periodic dynamics of the concentration oscillates between turning curves, and we defined a measure of their deviation from the equilibrium distributions that corresponds to the extent of the maximum ‘amplitude’ covered. This deviation asymptotically decays for high $D$ and $\tau$, and is highest for an intermediate skewness, although this last variation is weak.

Further work could involve revisiting previous studies of separating particles with different diffusivities (see [2]) in the light of these dynamical results. Another suggestion is to lift the restriction of equal ON and OFF durations and observing the effect of their ratio on dynamical features. The constraint of spatial periodicity in the dynamics may also be removed. This will allow studying the nature of the spatial aperiodicity and whether and how convergence to spatial periodicity (i.e. long-range order) occurs, analogous to the temporal observations carried out here.

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