# TRANSPORT IN RATCHET-TYPE SYSTEMS*,**

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Diffusion motion of overdamped Brownian particles in a spatially periodic asymmetrical potential and driven by a zero-mean time-periodic external force and zero-mean Gaussian white noise is considered. The influence of asymmetry of the spatial potential, amplitude of the driving force and intensity of the noise on an average translocation velocity of particles is analyzed. The adiabatic approximation for calculation of a stationary particle current is used and verified by comparison with results obtained from computer simulations of the process considered.

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## 1. Introduction

In generic cases, random perturbations, noises and fluctuations are reckoned to act destructively on physical (chemical, biological, economical, sociological) processes because such processes are less controllable than deterministic ones. *E.g.* voltage fluctuations can lead to damage of sensitive

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devices and instruments, random perturbations of electrochemical impulses can cause discharging of neurons. On the other hand, constructive influence of uncontrollable perturbations and noises is less obvious. Nevertheless, it is observed in all phenomena related to activation processes (*e.g.* diffusion limited chemical reactions) which have been studied for many decades [1]. New phenomena, in which noises can play positive role, are stochastic resonance [2] and Brownian ratchets [3].

In a wide sense, the ratchet is a system in spatially periodic but asymmetric potential driven by zero-mean forces, deterministic or/and stochastic ones. Feynman [4] used the "ratchet and pawl" to illustrate the meaning of the Second Law of thermodynamics and its implications. The aim of the Feynman considerations is an explanation, from the molecular point of view, for the fact that more that a certain amount of work cannot be extracted from a heat engine in going from one temperature to another and that if everything is at the same temperature then heat cannot be converted to work by means of cyclic processes. In another formulation it means that useful work cannot be obtained from equilibrium (thermal) fluctuations. Magnasco [5] reformulated this problem in terms of a system of overdamped Brownian particles in a periodic asymmetric (ratchet-like) potential and pointed out that: "the ratchet can extract energy (for free) out of the time correlated pieces of a colored (nonwhite) thermal bath" and "all that is needed to generate motion and forces in the Brownian domain is loss of symmetry and substantially long time correlations" [5]. It has been studied how the average translocation velocity of particles depends on stochastic characteristics of noises imposed, both correlated [6, 7] and white [3] noises. Another ratchet-type mechanism has been investigated, in which a spatially periodic potential is switched on and of periodically [8]. During the time-interval in which the potential is switched off, particles diffuse freely and symmetrically. During the following "on" period particles move towards minima of the potential and because the potential is asymmetrical, it pulls more particles in one direction than in the other. The result of this off-on switching is macroscopic drift of particles in a single direction. Modifications have been proposed: the switching is random and between two different non-zero potentials [9–11] or the barrier height of the potential is modulated [12]. The theoretical ideas have been realized experimentally [13] for a system of colloidal particles suspended in solution and exposed to an asymmetric dielectric potential. As it was shown in [13], the mean translocation velocity of particles depends on their size, suggesting applications in separation for particles of size which includes biological structures like cells, viruses, chromosomes, etc. Optical thermal ratchets were presented in [14] and a maximum of induced motion as a function of the modulation time of the spatial potential was observed.

Theoretical activity has been inspired by possible applications and explanation for some class of active processes in biochemical systems [15–20]. The effects of free-energy-driven oscillations and fluctuations on kinetics of chemical reactions, including enzyme catalysis, and the problem of extracting energy from the field of fluctuations were considered in [16]. Molecular motors were proposed to be modeled by ratchet-type systems in [18, 19]. Translocations of proteins into or across cellular membranes requires driving forces that can be Brownian (thermal) and directed motion is induced not by a temperature gradient but by chemical reactions. Different reactions on the cis and trans sides of a membrane correspond to a spatially asymmetric potential and can bias Brownian movements. As it is seen from above, processes in spatially periodic systems influenced by random perturbations (thermal noise, non-equilibrium fluctuations) are of great interest in almost all natural sciences starting from physics up to molecular biology ending.

In Section 2, we start with the description of the ratchet model which consists of Brownian particles in a spatially periodic potential and subjected to a time-periodic force. We present a general structure of solutions of the corresponding Fokker–Planck equation. In Section 3, we present an adiabatic approximation for calculation of a mean translocation velocity of particles or average current. In Section 4, we consider a specific model with the sawtooth potential and two-valued driving force. In the adiabatic approximation, we analyze the dependence of the current on parameters of the model such as an asymmetry parameter of the potential, amplitude of the external force and intensity of noise. Approximate results are compared with (almost exact) findings obtained from computer simulations of the stochastic Langevin dynamics. Section 5 contains summary.

## 2. Model and structure of solutions

We consider overdamped stochastic motion of particles in a spatially periodic potential and under the action of a time-periodical force. Our system is modeled by the equation [5, 21, 22]

$$\dot{x}_t = f(x_t) + F(t) + \xi(t)\,, \qquad f(x) = -\frac{dV(x)}{dx}\,, \tag{1}$$

where

$$V(x) = V(x+L)\,, \qquad F(t) = F(t+T) \tag{2}$$

is a spatially periodic potential with a period $L$ and an external driving time-periodic force of a period $T$, respectively. The external force is of zero average,

$$\langle F(t)\rangle = \frac{1}{T}\int_0^T F(\tau)d\tau = 0\,. \tag{3}$$

Furthermore, $\xi(t)$ is Gaussian white noise,

$$\langle \xi(t) \rangle = 0\,, \quad \langle \xi(t)\xi(s) \rangle = 2D\delta(t-s)\,, \tag{4}$$

with intensity $D$. This noise models interaction of the system with a thermal bath (the noise intensity $D$ is proportional to the temperature of heat bath).

The process $x_t$ defined by Eq. (1) is a nonstationary Markovian process and all probabilistic characteristics are determined by the Fokker–Planck equation for a conditional (transition) probability distribution. A one-dimensional probability distribution $p(x,t)$ obeys the same Fokker–Planck equation,

$$\begin{aligned} \frac{\partial}{\partial t}p(x,t) &= -\frac{\partial}{\partial x}(f(x)+F(t))p(x,t) + D\frac{\partial^2}{\partial x^2}p(x,t) \\ &\equiv K(x,t)p(x,t)\,. \end{aligned} \tag{5}$$

The Fokker–Planck operator $K(x,t)$ is periodic in space and time variables,

$$K(x,t) = K(x+L, t+T) \tag{6}$$

and Eq. (5) is invariant under discrete space and time translations. It implies that the operator $K(x,t)$ commutes with the translation operators $O_L$ and $U_T$ defined by the relations

$$O_L W(x,t) = W(x+L,t)\,, \qquad U_T W(x,t) = W(x,t+T)\,, \tag{7}$$

for an arbitrary function $W(x,t)$. Therefore the solutions of Eq. (5) can be presented as a linear combination of eigenfunctions of the operator $O_L U_T$ (note that $[O_L, U_T] = 0$). The eigenfunctions $\varphi_k(x,t)$ of the space-translation operator $O_L$ are of the Bloch-type form [22, 23],

$$\begin{aligned} \varphi_k(x,t) &= \exp\left(\frac{2\pi i k x}{L}\right) v_k(x,t)\,, \\ v_k(x,t) &= v_k(x+L,t)\,. \end{aligned} \tag{8}$$

If we require the solutions to be bounded for large $x$, values of the index $k$ must be real and then they can be restricted to the first Brillouin zone.

The eigenfunctions $\psi_n(x,t)$ of the time-translation operator $U_T$ are the Floquet-type solutions [24],

$$\begin{aligned} \psi_n(x,t) &= \mathrm{e}^{-\nu_n t} w_n(x,t), \\ w_n(x,t) &= w_n(x,t+T)\,, \end{aligned} \tag{9}$$

with the Floquet eigenvalues $\nu_n$ which are complex numbers. So, a general structure of solutions of Eq. (5) can be written in the form

$$p(x,t) = \sum_n \int dk\, c_n(k) \mathrm{e}^{-\nu_n t} \exp\left(\frac{2\pi i k x}{L}\right) u_{nk}(x,t)\,,$$
$$u_{nk}(x,t) = u_{nk}(x+L, t+T)\,, \tag{10}$$

where the expansion coefficients $c_n(k)$ are determined by the initial distribution $p(x,0)$.

For calculating mean values of quantities periodic in $x$, only periodic solutions

$$p(x,t) = p(x+L,t) \tag{11}$$

are needed and it restricts the values of the index $k$ to $k = 0$ only. Then

$$p(x,t) = \sum_n c_n \mathrm{e}^{-\nu_n t} u_n(x,t)\,,$$
$$u_n(x,t) = u_n(x+L, t+T)\,. \tag{12}$$

Because of periodicity, $p(x,t)$ is normalized in the period interval,

$$\int_0^L p(x,t)dx = 1\,. \tag{13}$$

For long times, as $t \to \infty$, the process $x_t$ in (1) tends to a stationary (or asymptotic) state that, because of the periodicity of the force $F(t)$, is time-dependent. Therefore the stationary (asymptotic) distribution $P_{\rm st}(x,t)$ is time-dependent and periodic in time. As a consequence, it can be presented by the Fourier series of time,

$$P_{\rm st}(x,t) = \sum_{n=-\infty}^{\infty} p_n(x) \exp\left(\frac{2\pi i n t}{T}\right)\,,$$
$$p_n(x) = p_n(x+L)\,. \tag{14}$$

The transport properties of the system (1) are determined by the probability current $J(x,t)$, which is given by the relation

$$J(x,t) = \big(f(x) + F(t)\big)p(x,t) - D\frac{\partial}{\partial x}p(x,t)\,. \tag{15}$$

In particular, the drift velocity

$$\langle v(t)\rangle = \langle \dot{x}_t \rangle = \langle f(x_t) + F(t) + \xi(t)\rangle$$
$$= \int_0^L dx \big(f(x) + F(t)\big)p(x,t) = \int_0^L dx J(x,t)\,, \tag{16}$$

where the expression (15) and spatial periodicity of $p(x,t)$ have been utilized.

The average probability current $J$ is defined as

$$J = \lim_{t\to\infty} \frac{1}{TL} \int_t^{t+T} dt \int_0^L dx J(x,t) \tag{17}$$

and this is the quantity of main interest. Unfortunately, this general method of analysis of transport properties of systems is difficult for applications and rather quantitative results can be obtained with the help of numerical calculations.

## 3. Adiabatic approximation

Analytical results for expectation values of the translocation velocity of particles or average probability current can be obtained approximately in some limiting cases. One of often used approximations is the adiabatic approximation. This approximation has been applied in almost all approaches for analysis of time-dependent processes in which hierarchy of time-scales exists. To profit by this method for the problem considered, let us assume that the $T$-periodic force $F(t)$ is a slowly varying function of time and hence

$$T \gg t_c\,, \tag{18}$$

where $t_c$ defines a characteristic time-scale of the deterministic system when $F(t) = 0$. It may be a relaxation time of the system to the equilibrium state (to the position of local minimum of the potential $V(x)$). It is argued that if (18) is fulfilled then for stationary states, as $t \to \infty$, $F(t)$ can be treated in Eq. (5) as a constant $F$, the distribution $p(x,t) \to p(x)$ and the current $J(x,t) \to J_a = \text{const.}$. Then from Eq. (15) it follows that

$$J_a = \big(f(x) + F\big)p(x) - D\frac{d}{dx}p(x) \equiv J_a(F)\,. \tag{19}$$

Two conditions, periodicity of $p(x)$ and its normalization over the period $L$ (*cf.* Eqs (11) and (13)), determine $J_a$ and the integration constant $N$ in (19). By eliminating the integration constant $N$, we get the following expression for the current [3, 23]

$$J_a(F) = D(1-\mathrm{e}^{-FL/D}) \left( \int_0^L dx \int_x^{x+L} dy \exp\left( \frac{V(y) - V(x) - (y-x)F}{D} \right) \right)^{-1}. \tag{20}$$

The average probability current $J$ and the mean translocation velocity $\langle v \rangle$ of particles can be obtained in this approximation from the following relations [5]

$$J = \frac{1}{T} \int_0^T J_a(F(t)) dt\,, \qquad \langle v \rangle = L\, J\,. \tag{21}$$

Let us notice that if $F = 0$ then $J = 0$ and for the systems driven by white noise and being only in spatially periodic potentials, current is zero and there is no transport in the system.

## 4. Specific model

To be more concrete, let us consider the following specific model. The spatially periodic potential $V(x)$ has the sawtooth form [5] (see Fig. 1),

$$V(x) = \begin{cases} \frac{A}{\eta} x, & \text{for } x \in [0, \eta] \bmod L = 1, \\ \frac{A}{1-\eta}(1 - x), & \text{for } x \in [\eta, 1] \bmod L = 1, \end{cases} \tag{22}$$

where $A > 0$ is potential barrier height and $\eta \in (0, 1)$ measures asymmetry of the potential ($\eta = 1/2$ corresponds to the symmetric case). The force $f(x)$ related to this potential has two values,

$$f(x) = \begin{cases} f_1 = -\frac{A}{\eta}, & \text{for } x \in [0, \eta] \bmod L = 1, \\ f_2 = \frac{A}{1-\eta}, & \text{for } x \in [\eta, 1] \bmod L = 1. \end{cases} \tag{23}$$

The time-periodic force $F(t)$ is chosen as (*cf.* Fig. 2)

$$F(t) = F \text{sign}[\sin(2\pi t/T)], \quad F > 0\,. \tag{24}$$

This force takes two values $F$ and $-F$ with frequency $\omega = 2\pi/T$. The mean value of $F(t)$ over one period is zero. The average current in the adiabatic approximation reads

$$J = \tfrac{1}{2}\big(J_a(F) + J_a(-F)\big)\,. \tag{25}$$

A closed expression for $J$ can be obtained [5], but here we visualize the dependence of the current on the parameters of the model in Figs 3–5. The system has two thresholds $f_1$ and $f_2$. When the thermal noise is absent (it corresponds to zero thermostat temperature) and the force $F(t)$ acts on the system then in the stationary regime there is a net particles flux only if $F > \min(-f_1, f_2)$ and the potential $V(x)$ is asymmetrical. The influence of asymmetry $\eta$ of the spatially periodic potential $V(x)$ on magnitude of

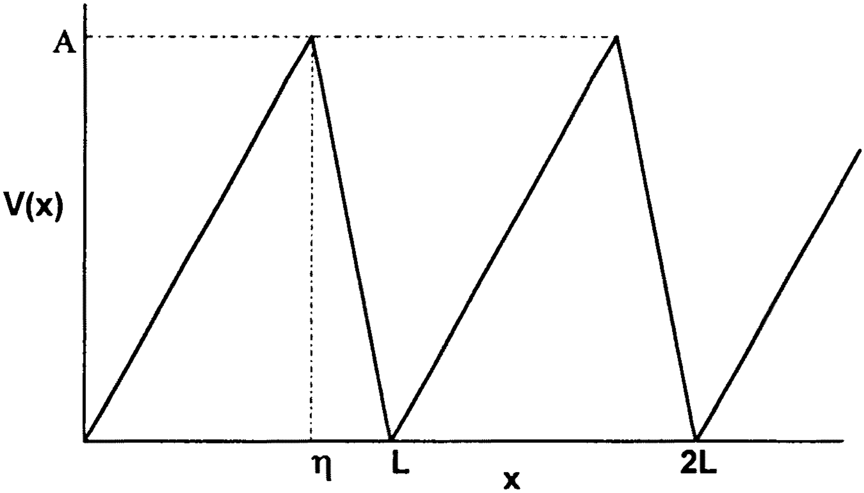


Fig. 1. The spatially periodic sawtooth potential $V(x)$ of period $L$, amplitude $A$ and asymmetry $\eta$.

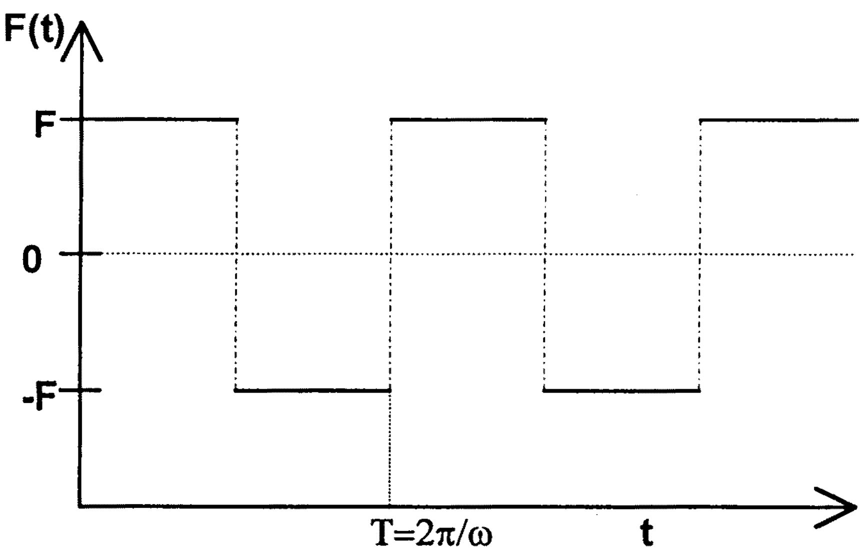


Fig. 2. The driving force $F(t) = F\text{sign}[\sin(2\pi t/T)]$.

current is depicted in Fig. 3. If $\eta = 1/2$ then $J = 0$. If $\eta > 1/2$ then $J > 0$ and vice versa. The greater asymmetry the greater current.

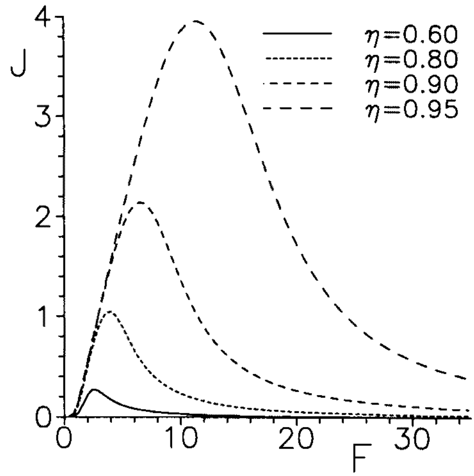


Fig. 3. Dependence of the average current $J$ on the driving amplitude $F$ for the noise intensity $D = 0.1$, the barrier height $A = 1$ and various values of the asymmetry parameter $\eta$ (the adiabatic approximation).

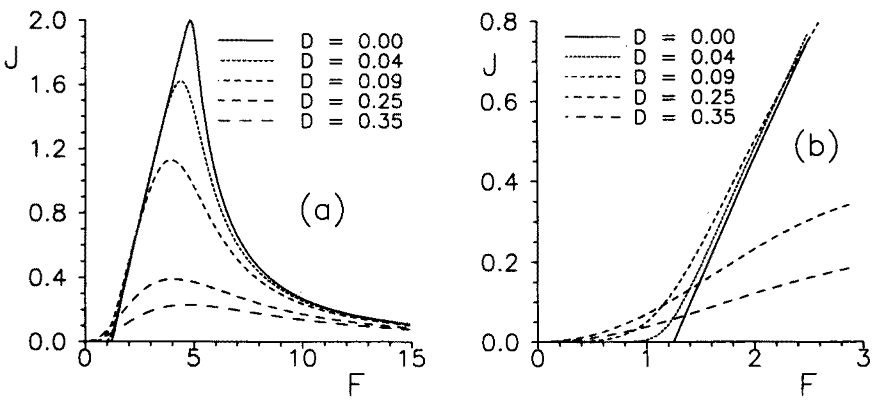


Fig. 4. Dependence of the average current $J$ on the driving amplitude $F$ for the barrier height $A = 1$, the asymmetry parameter $\eta = 0.8$ and various values of the noise intensity $D$ (the adiabatic approximation).

The dependence of the current on the amplitude $F$ of the external time-periodic force $F(t)$ for various noise intensities $D$ and fixed asymmetry $\eta = 0.8$ is presented in Fig. 4. The threshold values are $f_1 = -1.25$ and $f_2 = 5$. If the driving amplitude $F$ is below the threshold $-f_1$ then $J = 0$ for $D = 0$. If $D > 0$ then $J > 0$ and noise induces transport (*cf.* Fig. 4(b)). The maximal current is observed for the noiseless system (solid line), when

$D = 0$ and for value of $F$ that is equal exactly to the second threshold, $F = f_2 = 5$. For larger force amplitude, noise causes abatement of current. Let us note that there is an optimal value of the noise intensity $D$ for which current is maximal when $F < -f_1$ (see Fig. 5(a). Even for $F > -f_1$, the optimal value of $D$ maximalizing $J$ can be observed up to a certain value of $F$ above which noise is destructive (Fig. 5).

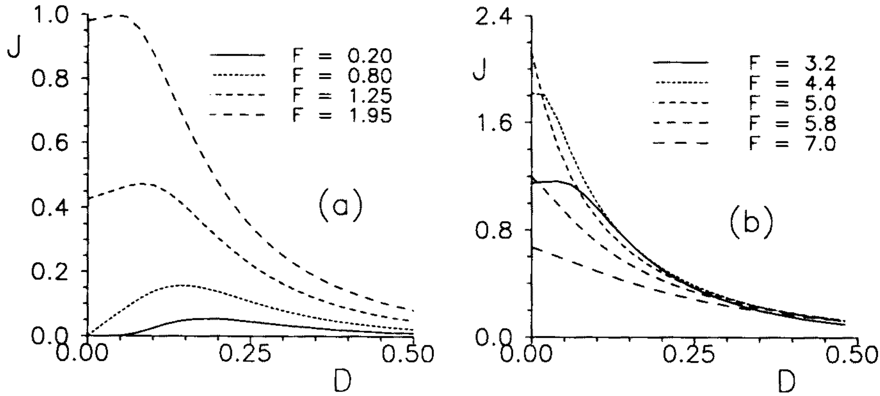


Fig. 5. Dependence of the average current $J$ on the noise intensity $D$ for the barrier height $A = 1$, the asymmetry parameter $\eta = 0.8$ and various values of the driving amplitude $F$ (the adiabatic approximation).

To justify correctness of the adiabatic approximation for this model, numerical simulations of the Langevin dynamics (1) with (23) and (24) have been carried out. An advantage of computer simulations of the stochastic differential equation (1) is the possibility to obtain quantitatively almost exact results independently on forms of the functions $V(x)$ and $F(t)$. Simulations were done by the same method as in [25]. Starting from random initial positions $x(t_0)$, we solved Eq. (1) using the Box–Muller method for generating random deviates with a normal distribution [26]. We carried out $10^6$ iterations with the step $h = t_n - t_{n-1} = 0.001\,\mathrm{s}$. The mean translocation velocity $\langle v \rangle$ of particles was evaluated as an arithmetical average of velocities $v_n = \Delta x/\Delta t$, where $\Delta x = x(t_n) - x(t_0)$ and $\Delta t = t_n - t_0$. Then from (21) we could calculate the current $J$. Results and comparison with the adiabatic approximation are presented in Fig. 6 for the noise intensity $D = 0.04$. The relaxation time $t_c$ in (18) is $t_c = 0.64$. It is the maximal time to reach a point of the potential minimum for the deterministic counterpart when $F(t) = 0$. We can notice very good preciseness of the adiabatic-limit results with simulations for the period $T = 120 \gg t_c = 0.64$ (*cf.* Fig. 6(a)). For $T = 10$, Fig. 6(b), the adiabatic approximation is still good. Even for $T = 1$, it gives qualitatively the same shape of $J$ although the adiabatic approximation overestimates the maximal exact value of the current which is also shifted to the right. For small values of $T$ (Fig. 6(d)), a new effect can be detected, namely, the current has several local extrema. A similar effect has been observed for another ratchet model [21]. The adiabatic approximation does not predict the existence of these extrema and it fails for large frequencies of the driving force.

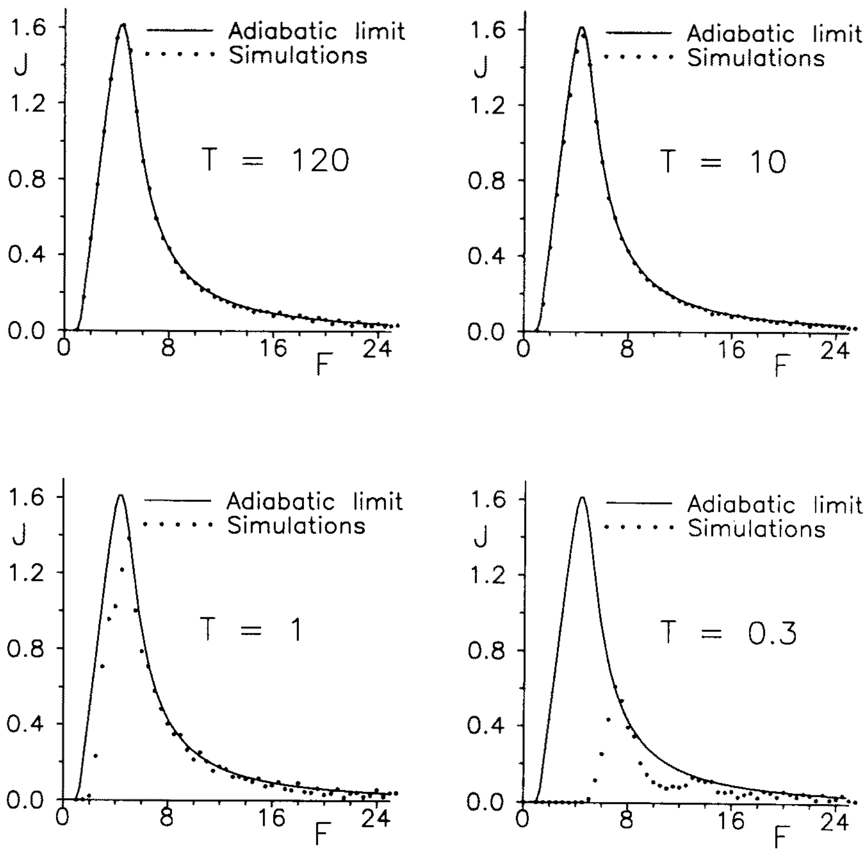


Fig. 6. Comparison of the adiabatic approximation for the current $J$ with computer simulation results for $D = 0.04$, $A = 1$, $\eta = 0.8$ and for various period $T$ of the driving force $F(t)$ in (24): (a) $T = 120$; (b) $T = 10$; (c) $T = 1$; (d) $T = 0.3$.

## 5. Summary

We presented one special type of ratchet models. For this model, transport is generated by the external time-periodic force $F(t)$ of zero-mean, $\langle F(t)\rangle = 0$ over one period. If $F(t) = 0$ then expectation value of the particle velocity is zero. It is demonstrated that thermal (Gaussian white) noise can play a positive role in two-fold sense:

*(i)* If amplitude $F$ of the driving force $F(t)$ is below the threshold determined by the form of the potential $V(x)$ so that the current $J = 0$ for a deterministic system ($D = 0$), then noise induces transport: $J \neq 0$ if $D > 0$, see Fig. 4(b).

*(ii)* If $F$ is above the threshold so that $J \neq 0$ even for $D = 0$, under right conditions (*i.e.*, for some range of values of parameters of the model) noise enhances the current: $J(D) > J(0)$, *cf.* Fig. 5.

Analytical formulas for the current can be obtained in some limiting cases as *e.g.*, in the adiabatic limit when the period $T$ of the driving force is much larger than the characteristic (relaxation) time $t_c$ of the deterministic counterpart. For $T < t_c$, a new effect is observed: several local extrema of the current as a function of driving amplitude occur. It cannot be described in the frame of the adiabatic approximation.

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