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Modeling the Jump-like Diffusion Motion of a Brownian Motor by a Game-Theory Approach: Deterministic and Stochastic Models

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Methods of paradoxical games are used to construct a stochastic hopping model of Brownian ratchets which extends the well-known analogous deterministic model. The dependencies of the average displacements of a Brownian particle in a stochastic ratchet system on a discrete time parameter are calculated, as well as the dependencies of the average ratchet velocity on the average lifetimes of the states of the governing dichotomous process. The results obtained are compared with both the results of modeling a similar deterministic model and the results of a known analytic description. While for the hopping analogue of the deterministic on-off ratchet, the time dependence of the displacement contains periodically repeated hopping changes when the potential is switched on and plateau of the diffusion stage of the motion when it is switched off, the stochastic dependencies, that are of an averaged character, are monotonous and do not contain jumps. It is shown that, with other things being equal, the difference in the results for the hopping ratchet model driven by the stochastic and deterministic dichotomous process of switching the potential profiles (game selection) is more pronounced at short lifetimes of the dichotomous states and vanishes with their increase.

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1. Introduction

The study of a controlled directed nanoparticle transport along spatially periodic structures is one of the topical problems of modern nonequilibrium statistical physics [1-4], with numerous applications, in, for example, design of nanoscale mechanisms of various complexity [5-7], description of intracellular transport [8-10], etc. Here, it is worth to speak of the ratchet effect (also termed the motor effect), which can be defined as the phenomenon of the appearance of a directed nanoparticle current as a result of introducing nonequilibrium unbiased fluctuations into a system, spatially and/or temporally asymmetric. The theory of Brownian motors describes this phenomenon, operates with a large number of models, and includes various

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approximations that allow analytical descriptions of both particular systems and general models that are valid for large classes of motor systems [1-3]. The motion of a Brownian particle in the field created by a fluctuating spatially periodic potential of a given shape is generally described by the Klein–Kramers equation [11] which is simplified to a description based on the Smoluchowski equation, if the nanoparticle mass can be considered negligibly small [3]. At low temperatures (the predominance of the values of potential barriers in comparison with the thermal energy), the so-called kinetic approach will be effective and rather simple. In it, the consideration of the continuous nanoparticle motion in the field of the spatially periodic potential is replaced by accounting for particle jumps between selected points (discrete "nodes") on the spatial period of the potential [12]. The redistribution of the node populations (which means the appearance of a directed hopping motion) under the introduction of fluctuations into the system can be calculated by solving the Pauli kinetic equation [13]. In this approach, the number of nodes normally corresponds to the number of wells on the period of the potential profile, in which the motion occurs, while the characteristics of the barriers are set using the rate constants of transitions between nodes. Hopping models of diffusion processes are of interest because they allow one to use original approaches and nonstandard analogies for modeling the ratchet effect, for example, the methods of Parrondo's paradoxical games [14]. In ratchet models, non-equilibrium fluctuations are often introduced into a system using a dichotomic process that switches two spatially periodic asymmetric potential profiles or states (here A and B). The switching can occur at regular intervals (deterministic process) or in a random manner (stochastic process characterized by the average lifetimes of the potential profiles). The first method is more typical for artificial nanomechanisms (see, for example, [15, 16]); the second one for natural protein motors, in which fluctuations of the effective potential profile occur due to the cyclic occurrence of the chemical reaction of ATP hydrolysis [8-10, 17], or for nanomechanisms, in which a random number generator, chemical reactions, or laser pumping are used to switch the states (as, e.g., in photomotors [18]). Consideration of the high-temperature ratchets [19] showed that, all other things being equal, the manner in which the potentials are switched significantly affects the characteristics of the ratchet effect: Its intensity (the maximum motor velocity) is higher for deterministic ratchet systems, while for stochastic ratchet systems, the fluctuation frequency range is wider, allowing, obviously, more degree of freedom in controlling the motor motion. In previous works [20, 21], we used the game-theory techniques to construct hopping models of deterministic Brownian motors with a double-well potential profile. There we have also studied the conditions under which controlling the direction of the particle current becomes possible. Stochastic game models with a discrete time parameter were then not involved. Since the comparison of deterministic and stochastic ratchet systems frequently give general theoretically interesting results (allowing to expand the understanding the mechanisms of generation of directed motion at the level of elementary acts of the diffusion process), which, in addition, has predictive value for future experimental applications, in this article we have filled this gap. Moreover, the method of theoretical research proposed here can be used as an alternative quick way to obtain the main characteristics of a Brownian motor without analytical calculations in cases where conditions arise under which the kinetic description is valid. The structure of the paper is the following. In Section 2, a theory of a stochastic dichotomic process with a discrete time variable is presented, on the basis of which, in Section 3, the relations for the average velocity of a hopping Brownian motor with an asymmetric double-well potential are obtained, and their deterministic analogs are also given. Section 4 presents the algorithm and the results of numerical modeling of the Brownian motor in the deterministic and stochastic description; the obtained results are summarized in Section 5.

2. Stochastic dichotomous process with a discrete time variable

Consider a system the state of which randomly alternates between A and B (see Fig. 1a). A time variable can be considered discrete, so it will be convenient to define it as the product $t = k\Delta t$, where Δt is the time step, and the integer variable k can take values 0, 1, 2, ... Assume that at $t = 0$ (corresponds to $k = 0$) the system was in the state A, and denote the probabilities of finding the system at arbitrary t in states A and B as $P_A(t)$ and $P_B(t)$, respectively; $P_A(t) + P_B(t) = 1$ and $P_A(0) = 1$. Additionally, let $P_{A\to B}$ and $P_{B\to A}$ be the probabilities of $A \to B$ (direct) and $B \to A$ (inverse) transitions; the corresponding probabilities for the system to remain in these states will then be $(1-P_{A\to B})$ and $(1 - P_{B\to A})$. We will apply the master equation for the probability that the system is in the state A at $t + \Delta t$,

$$P_A(t + \Delta t) = P_{B\to A}P_B(t) + (1 - P_{A\to B})P_A(t). \quad (1)$$

Equation (1) can be treated as a recurrent equation of the form $x_{k+1} = a + bx_k$, the solution of which can be readily obtained algebraically. Since $P_A(0) = 1$, the solution to Equation (1) is as following:

$$P_A(t) = \frac{P_{B\to A}}{P_{B\to A} + P_{A\to B}} + \frac{P_{A\to B}}{P_{B\to A} + P_{A\to B}} \times (1 - P_{B\to A} - P_{A\to B})^k. \quad (2)$$

In Section 3, we will use this solution obtained for the stochastic dichotomous process to check the quality of the numerical simulation results for the stochastic ratchet effect. Next, let us show that in the limit of continuous time variable ($\Delta t \to 0$), Equation (1) and its solution (2) tend, respectively, to the known equation and solution. Subtraction of Equation (2) for $P_A(t)$ from Equation (1) and subsequent division of the result by the increment Δt gives the following equation:

$$\frac{P_A(t + \Delta t) - P_A(t)}{\Delta t} = \gamma_B P_B(t) - \gamma_A P_A(t), \quad (3)$$

in which the quantities $\gamma_B = P_{B\to A}/\Delta t$ and $\gamma_A = P_{A\to B}/\Delta t$ are interpreted as the rate constants for transitions between the states (the average frequencies of potential switching), and $t_A = 1/\gamma_A$ and $t_B = 1/\gamma_B$ are the average lifetimes of the states A and B, respectively. In the limit $\Delta t \to 0$, Equation (3) becomes the master equation for the probability $P_A(t)$ as a function of continuous time variable

$$\frac{dP_A(t)}{dt} = \gamma_B P_B(t) - \gamma_A P_A(t), \quad (4)$$

the solution of which takes on the following form [22, 23]

$$P_A(t) = \frac{\gamma_B}{\Gamma} + \frac{\gamma_A}{\Gamma} e^{-\Gamma t}. \quad (5)$$

Here $\Gamma = \gamma_A + \gamma_B$ is the inverse correlation time of the dichotomous process. Let us show that the solution (5) follows from its discrete analogue (2). The deriving will include the relations $P_{B\to A} + P_{A\to B} = \Gamma\Delta t$ and $k = t/\Delta t$; then in the limit $\Delta t \to 0$, we obtain the relation $(1 - P_{B\to A} - P_{A\to B})^k = (1 - \Gamma\Delta t)^{t/\Delta t} \underset{\Delta t\to 0}{\to} e^{-\Gamma t}$ which, being substituted into (4), gives the result (5).

Summarizing, the master equation (1) and its solution (2) are discrete analogues of the Equation (4) and its solution (5) for the continuous time variable, respectively. At small values of Δt or long lifetimes $t_A(t_B)$, the probabilities $P_{A,B}(t)$ corresponding the discrete and continuous time variable will be close to each other. Hence, the features of a Brownian motor with discrete lifetimes can be distinguished at sufficiently small values $t_A(t_B)$.

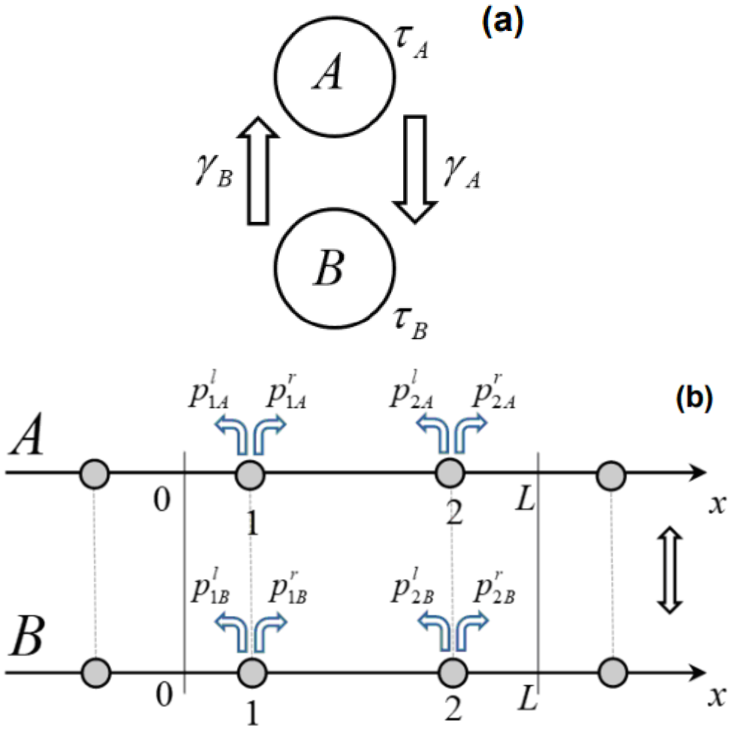

FIG. 1. Schematic representation of (a) two states of a dichotomic process, characterized by the lifetimes τ_A, τ_B and the average frequencies γ_A, γ_B at deterministic and stochastic switching of the states, respectively, and (b) a jumping model of a Brownian motor with a periodic double-well potential.

3. Hopping model of a Brownian motor with a double-well potential

A Brownian motor is a nanosystem in which a particle directed motion, translational or rotational, is induced by introducing nonequilibrium fluctuations into the system provided that it is spatially and (or) temporally asymmetric. Let us consider a model in which a nanosystem is alternately in two states, A and B. State A corresponds to a spatially periodic (with period L) asymmetric double-well potential profile while the state B corresponds either to free diffusion (when considering the so-called on-off ratchet) or to another spatially periodic (with the same period L) potential profile (if we talk about a more general pulsating-ratchet model). The alternation of the states is either a dichotomous deterministic or dichotomous stochastic process. In the state A, we choose the locations of potential wells in the interval $(0, L)$ at nodes 1 and 2 (see Fig. 1b); $p^l_{1(2)A}$ and $p^r_{1(2)A}$ will notate the probabilities that a particle, being initially located at the node 1 (2), makes a jump to the nearest leftward and rightward potential well, respectively. These probabilities mean the escape probabilities over the potential barrier ΔV and are proportional to the exponential factors of the Arrhenius law, $\exp[-\beta\Delta V]$, where $\beta = (k_B T)^{-1}$. In the state B, we similarly associate the particle escape probabilities $p^{l(r)}_{1(2)B}$ with the same nodes 1 and 2; in the case of free diffusion the probabilities $p^{l(r)}_{1(2)B}$ can be defined as [21]

$$p^l_{1B} = p^r_{1B} = c_1/2, \quad p^l_{2B} = p^r_{2B} = c_2/2, \qquad (6)$$

the ratio c_1/c_2 being determined by the geometrical arrangement of nodes 1 and 2.

In addition, the values of the probabilities must satisfy the detailed-balance condition (the condition for the equilibrium in each state), imposed on the kinetic characteristics:

$$p^l_{1A(B)}p^l_{2A(B)} = p^r_{1A(B)}p^r_{2A(B)}. \quad (7)$$

For a deterministic dichotomous process, the states A and B being characterized by the lifetimes $\tau_A\Delta t$ and $\tau_B\Delta t$ (τ_A and τ_B are integers), the average rate of change in population of nodes 1 and 2 in the adiabatic mode is given by the following relation [24]

$$< v_d >= \frac{2[p^r_{1A}/p_{1A} - p^r_{1B}/p_{1B}]}{\tau_A + \tau_B}[R_{1B} - R_{1A}][1-(1-p_{1A}-p_{2A})^{\tau_A}][1-(1-p_{1B}-p_{2B})^{\tau_B}],$$
$$R_{1A(B)} = \frac{p_{2A(B)}}{p_{1A(B)} + p_{2A(B)}}, \quad p_{1(2)A(B)} = p^l_{1(2)A(B)} + p^r_{1(2)A(B)}. \quad (8)$$

For a continuous time variable, the average velocity of a Brownian motor (the average rate of change in population of the nodes) can be found by using the electroconformational model [25], within which the velocity in case of a deterministic (index d) and stochastic (index s) dichotomous governing process takes on the following form:

$$< \tilde{v}_{s,d} >= \frac{\gamma_A\gamma_B}{\Gamma}(\frac{p_{2B}}{\Sigma_B} - \frac{p_{2A}}{\Sigma_A})\varphi_{s,d}\,,$$
$$\Sigma_{A(B)} = p_{1A(B)} + p_{2A(B)}\,,$$
$$\varphi_s = \left(1 + \frac{\gamma_A}{\Sigma_A} + \frac{\gamma_B}{\Sigma_B}\right)^{-1},$$
$$\varphi_d = \frac{2\sinh[\Sigma_A/(2\gamma_A)\,]\sinh[\Sigma_B/(2\gamma_B)\,]}{\sinh[\Sigma_A/(2\gamma_A)\ + \Sigma_B/(2\gamma_B)\,]}\,. \quad (9)$$

In the next chapter, we will use Eqs. (8) and (9) to analyze the accuracy of the values of the motor average velocity obtained by numerical modeling.

4. Modeling within the game theory approach

Modeling the hopping diffusion motion in terms of the game theory has been carried out by using the approach described in [20]. According to it, a particle displacement relative to its initial position at time $t = 0$ is associated with a change (increase or decrease) in the capital $n(t)$ of a player, and a single act of particle hopping motion in the state A or B is interpreted as tossing a dice when playing game A or B and, accordingly, a possible win or loss. It is logical to partition the modeling procedure into two subprocedures (units): (i) capital change within one of the states A or B (Fig. 1b), according to the rules of the game A (B), and (ii) switching the states (games) (Fig. 1a). Further we will consider each of the subprocedures. When a game is selected (the index A (B) is known), each step is simulated using a random variable generating procedure: Having uniformly distributed values over the interval $(0, 1)$, a random variable, ξ, is created at each step. Depending on the values which ξ takes, there exists three possibilities: (i) the capital increases by unity (ξ values are within the interval $(0, p^r_{1(2)A(B)}]$), (ii) the capital decreases by unity (ξ values are within the interval $(p^r_{1(2)A(B)}, p^r_{1(2)A(B)} + p^l_{1(2)A(B)}]$), and (iii) the capital remains unchanged (ξ values are within the interval $(p^r_{1(2)A(B)} + p^l_{1(2)A(B)}, 1)$). Which set of probabilities for nodes numbered 1 or 2 will be valid in each specific case is determined through the parity of the current (integer) value of the capital $n(t)$ (or, in the case of a large number of wells per period, of the function of the division remainder, $n(t) \mod N$). Which game, A or B, is being played at current time is determined in the second subprocedure which simulates the game alternating. In the model of the deterministic dichotomous process, in each of the games, the number of steps (the number of tossing the dice), equal to the integer lifetime $\tau_{A(B)}$ of the state is simulated; after the system passes this number of steps, the games are switched. When modeling the stochastic dichotomous process, before each tossing the dice and changing the capital, an additional procedure determines whether there will be a change in the current game. Namely, an auxiliary random variable η is generated, its values η_n are uniformly distributed over the unit interval, $(0, 1)$. If η_n falls into the interval $(0, \gamma_{A(B)})$, the games are switched, otherwise (the value η_n is in the interval $[\gamma_{A(B)}, 1)$), we play the same game. Thus, the dichotomous switching of the games is realized by means of a simple loop counter, while the stochastic one – by means of the auxiliary random variable η at each step of the loop. The correct functioning of this part of the algorithm can be checked by comparing the averaged modeled dependence of the probability of finding the system in the states (games) A and B on t with analytical formula (2). In the review [26], one can find a systematic analysis of different factors which the ratchet motion direction depends on. For an on-off ratchet, one of the ways to affect the ratchet motion direction is to use a double-well potential, its minima being located at different distances from the location its highest barrier [27]. Parametrization of such a potential in terms of probabilities of transitions between the potential wells was performed in [21] (using the Arrhenius law, the values of transition probabilities are assign to the values of minima and maxima of the potential profile), the results of [21] were used here to construct the computational model. In the state B, which describes the free diffusion, the geometric arrangement of nodes 1 and 2 (determining motion direction) is characterized by different probabilities of the jump of particles from these nodes (in Eq. (6)). Let us denote by (a) and (b) the sets of parameter values associated, respectively, with the low-temperature ($\beta\Delta V = 2$) and high-temperature ($\beta\Delta V = 0.5$) ratchet operation modes. Then, according to [21], the parameterization of the corresponding potential profiles makes it possible to operate in the hopping model with the following sets of transition probabilities: (a) $p^l_{1A} = 0$, $p^r_{1A} = 0.1353$, $p^l_{2A} = 0.0183$, $p^r_{2A} = 0$, $c_1 = 1$, $c_2 = 1/3$; and (b) $p^l_{1A} = 0$, $p^r_{1A} = 0.6065$, $p^l_{2A} = 0.3679$, $p^r_{2A} = 0$, $c_1 = 1$, $c_2 = 1/3$. Figure 2 shows the averaged, over 3 million realizations (experiments), trajectories of capital accumulation for the deterministic (the solid curves with square markers) and stochastic (the dotted curves with round markers) dichotomous process. Figures 2a and 2b are related to the lifetimes values $\tau_A = \tau_B = 2$ and $\tau_A = \tau_B = 5$ (for deterministic dependencies) and the corresponding frequencies $\gamma_A = \gamma_B = 1/2$ and $\gamma_A = \gamma_B = 1/5$ (for stochastic dependencies); below we will indicate these sets of the time parameters as [2; 2] and [5; 5]. The obtained graphical results supplement the known deterministic results [21] with dependencies characteristic of ratchets with the stochastic alternating the states. In both figures, the upper pairs of the trajectories (calculated with the set (a) of the probability values and marked with open markers) demonstrate the increase in capital, or, in terms of the theory of Brownian motors, a rightward shift of particles. The lower pairs of trajectories (the set (b), filled markers), in their turn, demonstrate the decrease in capital and hence the corresponding particle motion to the left. From the Fig. 2, one can see that the periodic switching of the potentials at chosen times on the time period strictly reflects the directed motion mechanism: One can observe the periodic (steady-state) structure of the curves, the points at which the potential A is switched on (a jump) and the plateau – the diffusion stage

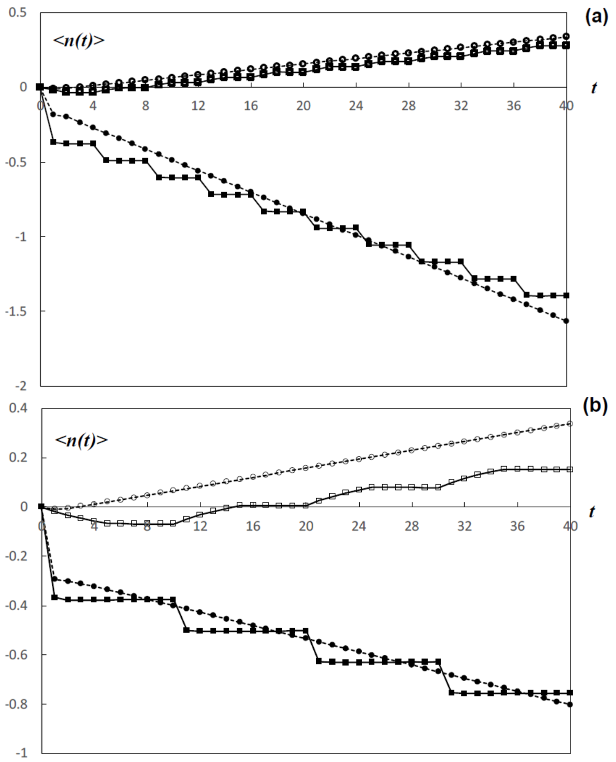

FIG. 2. Averaged (over 3 million realizations) trajectories of capital accumulation for the deterministic (solid curves with square markers) and stochastic (dotted curves with round markers) dichotomous process with time parameters [2; 2] (a) and [5; 5] (b). The curves with open and filled markers correspond to the low-temperature (a) and high-temperature (b) sets of parameters, respectively, in the model of nanoparticle motion in the double-well potential associated with each of the games.

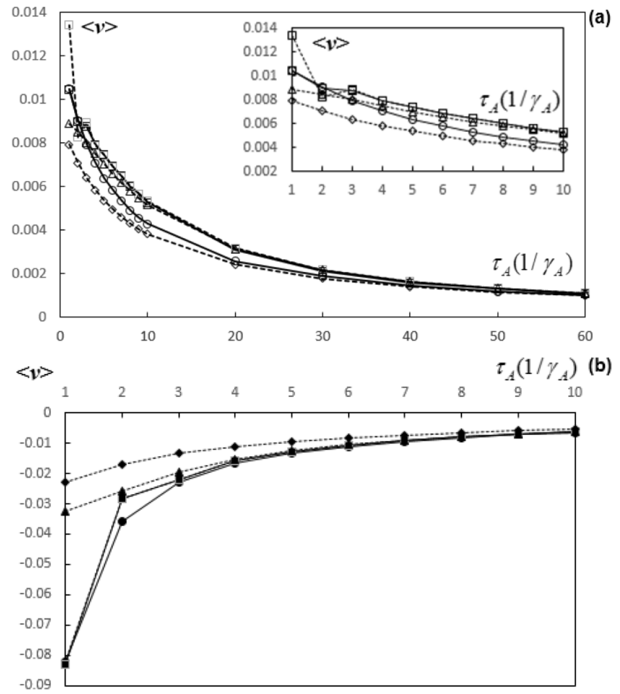

FIG. 3. Dependencies of the average motor velocity on the lifetime of the states $\tau_A = \tau_B$ ($\gamma_A = \gamma_B$) obtained by simulating games (solid curves with square and round markers) and calculated by formulas (8) (dashed curves with square markers) and (9) (dashed curves with triangular and rhombic markers). The curves with open and filled markers relate to the low-temperature parameter set (a) and the high-temperature parameter set (b); square and triangular markers mark dependencies arising at deterministic potential switching, round and rhombic markers at stochastic one. The insert details the behavior at small values of $\tau_A(1/\gamma_A)$.

B. Stochastic trajectories are averaged because of the random switching of the potentials In Figs. 3 and 4 we present the comparative dependencies of the average velocities on the lifetimes of the states A (B) [for the case of the deterministic switching the states (with $\tau_A = \tau_B$)] and on the reciprocal rate constants of transitions [for the case of stochastic switching the states (with $\gamma_A = \gamma_B = 1/\tau_A$)], obtained by numerical simulations and analytical formulas (8) and (9). Figure 3 compares features in high- and low-temperature behavior of deterministic and stochastic hopping-ratchet model of an arbitrary pulsating type. Figure 4 relates to the high-temperature deterministic and stochastic ratchets with equal probabilities of the state B (being somewhat a hopping analogue of an on-off ratchet with continuous time variable). Figures. 3a and 3b correspond, respectively, to the set (a) and (b) of the probability values. The curve calculated by formula (8) for discrete lifetimes of the states perfectly repeats the curve obtained by the simulation procedure. In the high-temperature operation mode of the Brownian motor (Fig.3b), the deterministic and stochastic dependencies (solid lines) differ only at small τ_A values and coincide as τ_A increases to 10,

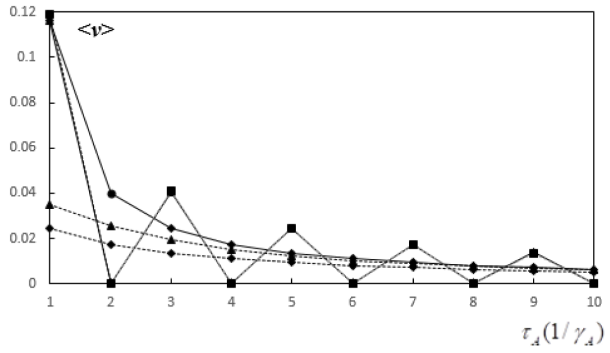

FIG. 4. Dependencies of the average motor velocity on the lifetime of the states $\tau_A = \tau_B$ ($\gamma_A = \gamma_B$) obtained by simulating games (solid curves with square and round markers) and calculated by formulas (8) (dashed curves with square markers) and (9) (dashed curves with triangular and rhombic markers); the A-state probabilities are given in the set (b), all the B-state probabilities are chosen 0.5. Square and triangular markers mark dependencies arising at deterministic potential switching, round and rhombic markers at stochastic one.

while in the low-temperature mode (Fig. 3a) these dependencies approach each other much more slowly (see the inset in Fig.3a). The performed simulation thus validates the conclusion made in Section 3 about the coincidence of the results of the both descriptions, continuous and discrete, at large τ_A values. The coincidence of the average-velocity values for stochastic and deterministic processes of the state switching at the point $\tau_A = 1$ follows from the fact that, at this τ_A value, the random scheme of the switching the states is impossible to be realized, because the equality $\gamma_A = \gamma_B = 1$ means that, with each tossing the dice, the switching reliably occurs.

The results presented in Fig. 4 are calculated with the set (b) of the state-A probability values and for the probabilities of the state B all chosen equal to 0.5 (that is, the state B was the free diffusion state, characterized by equal probabilities associated with all locations and directions). Then, for the deterministic switching the states characterized by equal lifetimes ($\tau_A = \tau_B$), the form of the dependence of the average velocity on τ_A is nontrivial: For even τ_A values, the velocity is equal to zero (the ratchet effect vanishes), while for odd τ_A values, it is nonzero (the ratchet effect can be observed). Moreover, being not in the thermodynamic equilibrium, the system demonstrates the zero average velocity; the currents exist but they are balanced when changing the states, such that the structures somewhat similar to beats or standing waves occur. Stochastic dependencies, for which the probabilistic processes have already been taken into account, are of a more standard form having no stopping points.

Similar to the dependencies in Fig. 3, the curves in Fig. 4 demonstrate perfect agreement between the results of numerical and analytical modeling for deterministic adiabatic switching the states (the solid and dashes curves with square markers). At the same time, the stochastic calculated and analytical (according to (9), for a continuous time variable) dependencies are different (the curves with round and rhombic markers), but they approach each other with the increase of the value of τ_A. The same approaching occurs with increase in τ_A value between the calculated curves obtained for the hopping model with the deterministic state switching and the curve by Eq. (9) of the deterministic ratchet model with the continuous time variable (the curves with square markers, oscillating, approach the curve with triangular markers). Thus, the simulation results are well confirmed by analytical dependencies.

5. Discussion and conclusions

In this work, we have continued and expanded the results of Refs. [20, 21] devoted to the application of game-theory models to study the nonequilibrium nanoparticle transport arising due to the ratchet effect. Using the technique proposed in Refs. [20,21], which was developed for modeling the hopping motion for deterministic Brownian ratchet models, a stochastic model was constructed that showed good agreement with the analytical description in the limiting cases.

The comparative description of the nanoparticle motion characteristics for models assuming the deterministic and stochastic switching the states has been performed; it demonstrated significant differences in dependencies of motion characteristics on time parameters. In the stochastic model, the process of switching the states is of a probabilistic nature, which is also reflected in the fundamentally different behavior of the trajectories of capital accumulation and the average ratchet velocity, if we compare this behavior with those of the same-name deterministic dependencies that have a periodic structure (Figs. 2 and 4). This difference is most pronounced at small values of the lifetimes of states (high frequencies of state switching), gradually decreases with their increase (see Fig. 3) and vanishes at large values of $\tau_{A(B)}$ (values of $t_{A(B)}$ corresponding to $t_{A(B)}$). The reason for such behavior of the average velocity is the transition of the system to the adiabatic operation mode, for which, as is well known, both models of potential switching, stochastic and deterministic, are actually equivalent. The proposed model was illustrated on two sets of probabilities of transitions between the nodes of the state B. Low-temperature (Figure 2) and high-temperature (Figure 3) dependencies, in addition to demonstrating the difference in the behavior of hopping ratchets with dichotomous stochastic and dichotomous deterministic algorithms of potential switching, confirm the predicted (see Ref. [21]) ability to control the direction of the nanoparticle current by setting the temperature regime of the ratchet operation. Analysis of the both models, in which all the values of the transition probabilities in the state B were chosen the same ($\tau_A = \tau_B$; the case can be called the hopping analogue of an on-off ratchet) (Figure 4), demonstrated the appearance of stopping points of the deterministic motor (zero average velocity) at even values of the lifetimes of states, which, however, do not arise for motors controlled by a stochastic dichotomous process.

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