A modified active Brownian dynamics model using asymmetric energy conversion and its application to the molecular motor system

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Abstract We consider a modified energy depot model in the overdamped limit using an asymmetric energy conversion rate, which consists of linear and quadratic terms in an active particle's velocity. In order to analyze our model, we adopt a system of molecular motors on a microtubule and employ a flashing ratchet potential synchronized to a stochastic energy supply. By performing an active Brownian dynamics simulation, we investigate effects of the active force, thermal noise, external load, and energy-supply rate. Our model yields the stepping and stalling behaviors of the conventional molecular motor. The active force is found to facilitate the forwardly processive stepping motion, while the thermal noise reduces the stall force by enhancing relatively the backward stepping motion under external loads. The stall force in our model decreases as the energy-supply rate is decreased. Hence, assuming the Michaelis–Menten relation between the energy-supply rate and the ATP concentration, our model describes an ATP-dependent stall force in contrast to kinesin-1.

Keywords Active Brownian particle · Overdamped motion · Flashing ratchet · Molecular motor

1 Introduction

Since the stepping motion of kinesin was first observed by a single-molecule experiment [1], similar discrete motions of various molecular motors have been reported [2–5]. Single-molecule techniques [6, 7] have shed light on the mechanisms of these tiny biological

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motors. Among various molecular motors, kinesin has been mostly studied and numerous fruitful findings have been reported. Kinesin-1 walks processively along a microtubule toward the plus end (defined as ‘forward’) for more than 100 steps using alternate binding heads on the microtubule in an asymmetric hand-over-hand manner. A force of 6–8 pN per step is generated by consuming one adenosine-triphosphate (ATP). Step size is known to be independent of the ATP concentration and external load and is about 8 nm, which corresponds to the axial length of one tubulin-dimer, the building block of the microtubule [1, 8–17]. In spite of the extensive single-molecule studies, how kinesin functions to generate the force for discrete translation on a single protofilament of the microtubule is not well understood, leaving many questions on, for instance, substeps, backsteps, and fraction of power stroke and diffusion to each step [10, 18–23].

Molecular motors convert chemical energy directly to mechanical work and hence are much different from the conventional macroscopic motors. To study the dynamics of molecular motors theoretically, a variety of models have been introduced. The rectified-diffusion model [24, 25] was suggested by assuming that a motor diffuses on a microtubule, and yielded only 1 pN of maximum force exerted against a viscous load. In a flashing-ratchet model [26–29], a motor diffuses on alternating ratchet potentials of different barrier heights and performs a unidirectional movement as a result. The flashing ratchet model can be converted to a powerstroke model [30–32] if a phase-shifted ratchet is introduced instead of a flat potential. In a hand-over-hand model [8, 12, 33] for motors with two heads, one head diffuses to find the next binding site while another binds to a microtubule supporting a load. There is strong experimental evidence for this model [14, 15, 34, 35]. Hence biological motors performing discrete unidirectional motion are believed to function in a combination of powerstroke and Brownian mechanisms.

In an active Brownian particle model [36], the particle is driven by an active force, which can perform mechanical work by converting internal energy stored in an energy depot. The model was firstly developed with a quadratic, and hence symmetric, energy conversion rate in the particle’s velocity. As a consequence of this symmetry, the magnitude of active driving force does not depend on a moving direction so that the active driving mechanism just facilitates a transport in a direction of the particle’s instantaneous movement. Within the symmetric active Brownian particle model, processive stepping motion in a realistic biological environment has not been described. The model has been studied extensively and applied successfully to various self-propelling processes [37–44]. The energy conversion rate was recently generalized [45] by adopting a polynomial of the particle’s position and velocity as a functional form of conversion rate. The symmetry of the original model is broken in the generalized model, yielding a rich variety of dynamical characteristics. For example, stepping motions similar to those observed in the processive molecular motors were observed in the absence of any potential with a carefully chosen conversion rate as a function of velocity up to the fourth order [45].

Applying the generalized active Brownian particle model to molecular motors is quite plausible because the model includes an active force and diffusion mechanism. The generalized model was more or less successful in capturing primary features of molecular motors such as forward/backward stepping and stalling against an external load when the energy conversion rate was assumed to be a polynomial up to the fourth order of the particle’s velocity [46]. However, four arbitrary parameters to be chosen properly are difficult to handle and in the stalling state the particle did not move at all instead of exhibiting equal numbers of forward and backward steps. Moreover, an effect of thermal fluctuation on the model was not investigated.

In this paper, we construct an active Brownian dynamics model with only two parameters in the energy conversion rate function and employ a flashing ratchet potential synchronized to a stochastic energy supply. We believe that this model itself is physically interesting though we adopt a molecular motor system as a background since the model can capture the processive stepping motion. Our energy conversion rate consists of two terms that are linear and quadratic in the particle's velocity. This is the simplest case of the generalized model. The linear term breaks a symmetry of energy conversion rate and alters the active driving mechanism. General aspects of this model will be discussed in detail elsewhere. Here, we confine ourselves to a particular choice of the two parameters in the conversion rate, which possibly yields a more or less proper description for kinesin motor dynamics. The input energy from ATP hydrolysis is assumed to be delivered via a pulse-like sequence of energy influx following the Poisson process with a finite ATP binding rate. A periodic ratchet potential is adopted in order to take into account an interaction between the motor molecule and the microtubule [29, 39]. The coupling strength is reported to be weak when the rear head undertakes a biased diffusional search for its forward binding site. On the other hand, the coupling becomes strong when the new front head binds to the microtubule after releasing an ADP [18, 47, 48]. Hence the interaction strength is not a constant during a one-step cycle. To consider this modulation of the potential strength, we assume that the modulation is synchronized with the stochastic energy supply in such a way that the ratchet potential is weak during the energy supply or strong otherwise.

We perform a one-dimensional active Brownian dynamics simulation to investigate the dynamical properties of an active particle such as the molecular motor. Due to a negligible inertia effect in the nano-world, we consider the overdamped dynamics of the motor in contrast to the standard energy depot model. We introduce a modified energy depot model where the energy conversion function is defined in terms of the instantaneous drift velocity to avoid the difficulty of defining velocity in the overdamped Langevin equation of motion in the presence of thermal noise [49]. Based on our modified model, effects of the thermal fluctuations as well as of the active force, external load, and energy-supply rate associated with the molecular motor are studied and analyzed in detail.

This paper is organized as follows. In Section 2, we introduce a modified energy depot model and apply the model to the kinesin motor system. In Section 3, results of the active Brownian dynamics simulation in the absence and presence of thermal noise are presented. Concluding remarks follow in Section 4.

2 A modified energy depot model

If a Brownian particle can store a supplied energy in its internal depot and convert an internal energy into mechanical work, then the motion of the Brownian particle is called active [37, 38]. From the conservation of energy in the depot, the internal energy $e(t)$ at time t can be described as [45, 46]

$$\frac{de}{dt} = q(x, t) - ce - d(x, v)e, \quad (1)$$

where $q(x, t)$ is the energy influx to the depot, c is the constant rate of internal energy dissipation, and $d(x, v)$ is the conversion rate of the internal energy into mechanical work. While the conversion rate is assumed to be symmetric as $d(x, v) \sim v^2$ in the original model

[37, 38], we consider an asymmetric conversion rate in order to mimic the stepping motion of a molecular motor.

The equation of motion for an active Brownian particle coupled to the energy depot is then written as

$$m \frac{dv}{dt} = -\gamma v + F_{\text{active}} + F + \zeta(t), \quad (2)$$

where m , v , γ are mass, velocity, and friction coefficient of the particle. F_{active} is the active force due to an energy transfer from the energy depot and F is the external force. $\zeta(t)$ is the Gaussian white noise, where $\langle \zeta(t) \rangle = 0$ and $\langle \zeta(t)\zeta(t') \rangle = 2\gamma k_B T \delta(t - t')$ with T being the temperature and k_B the Boltzmann constant. The external force F consists of two contributions,

$$F = f_L + f_M, \quad (3)$$

where f_L is the constant load that can be experimentally controlled via the force-feedback trap and f_M is the interaction between the motor and the microtubule. We do not consider a possibility of motor detachment from the microtubule.

Energy supply due to ATP hydrolysis—We model the energy influx as a sequence of random pulses at time $\{t_i, i = 1, 2, 3, \dots\}$ with finite duration t_c as

$$q(t) = \sum_i q_0 [H(t - t_i) - H(t - t_i - t_c)], \quad (4)$$

where q_0 is the energy supply rate and H is the Heaviside step function. An energy pulse corresponds to the hydrolysis of an ATP, which occurs repeatedly at a time interval λ . Since the amount of energy released from the hydrolysis of one ATP is about $25k_B T$ physiologically, we use $q_0 t_c = 25k_B T$ and assume $t_c = 3$ ms, yielding $q_0 = 25k_B T/3$ ms. The delivery of energy pulses is assumed to follow a Poisson process with a mean waiting time λ [42, 43]. We can then sample t_i from the exponential distribution of the waiting times as

$$P(t_i - t_{i-1}) = \frac{1}{\lambda} \exp\left(-\frac{t_i - t_{i-1}}{\lambda}\right). \quad (5)$$

Later, the time interval λ of the energy supply will be roughly interpreted as the ATP concentration using the Michaelis–Menten relation.

Active driving force—We assume that the energy conversion rate is the second-order polynomial of the velocity,

$$d(v) = a_1 v + a_2 v^2, \quad (6)$$

where the coefficients a_1 and a_2 are parameters determining the energy conversion mechanism of the motor. The active force is then given by

$$F_{\text{active}} = \frac{d(v)e}{v} = (a_1 + a_2 v)e. \quad (7)$$

The general mathematical and physical analysis and discussion of this asymmetric second-order model will be given elsewhere, and in this work, we consider only the case where both a_1 and a_2 are positive. In the model where $a_1 = 0$ [37–44], F_{active} has always the same direction as v and accelerates the motor in the direction of v in a symmetric manner. In the present model, on the other hand, there exists a regime of negative $d(v)$, i.e., $-a_1/a_2 < v < 0$, where the energy conversion can be inverted. That is, the mechanical energy can be

converted to the internal energy such as elastic energy of the motor molecule, for instance. In this regime, the active force can drive the motor to the forward direction even when the motor moves in the backward direction, which is not possible in the original symmetric model. Therefore, one can conclude that the positive a_1 facilitates the driving of the motor in the forward direction when $v > -a_1/a_2$.

Interaction between kinesin and microtubule—It is known that the interaction between the rear head of kinesin and the microtubule is strong until the ATP bound to the rear head hydrolyzes. After the hydrolysis, it becomes weak until the rear head swings to find the next binding site just after a new ATP binds to the front head. To reflect this, we consider an interaction between the motor and the microtubule as a time-dependent ratchet potential:

$$U(x, t) = \begin{cases} \frac{U_0(t)}{b}(x - nL) & \text{if } nL \leq x \leq nL + b \\ \frac{U_0(t)}{b-L}[x - (n+1)L] & \text{if } nL + b \leq x \leq (n+1)L \end{cases} \quad (8)$$

where n is an integer, b is the asymmetry parameter of the ratchet potential chosen as $L/3$, and L is the axial distance of a tubulin-dimer, 8 nm. $U_0(t)$ is the time-dependent potential strength defined in such a way that $U_0(t) = U_{\text{weak}}$ during the period of energy supply or $U_0(t) = U_{\text{strong}}$ otherwise. Hence the flashing is synchronized to the energy supply mechanism. The force due to the ratchet potential, f_M , can then be obtained as

$$f_M = -\frac{\partial U}{\partial x} \quad (9)$$

$$= \begin{cases} -\frac{U_0(t)}{b} & \text{if } nL \leq x \leq nL + b \\ \frac{U_0(t)}{L-b} & \text{if } nL + b \leq x \leq (n+1)L \end{cases} \quad (10)$$

which is a piecewisely constant force with alternating signs.

An overdamped limit—Since the very small mass ($\sim 10^{-22}\text{kg}$) of kinesin makes a negligible inertial contribution [49], we confine ourselves to an overdamped limit. Then velocity is not well-defined in the presence of thermal noise and hence the energy conversion rate cannot be determined. To keep the energy depot model consistent in the overdamped limit, it is necessary to define the energy conversion rate in an alternative way. For this purpose, we assume that the energy conversion mechanism is irrelevant to the thermal noise, since the time scale of thermal fluctuation is much smaller than the others. We define a drift velocity v_d as an instantaneous velocity in the absence of thermal noise:

$$v_d = \frac{f_L + f_M + a_1 e}{\gamma - a_2 e}, \quad (11)$$

where we restrict $\gamma > a_2 e$ since γ is sufficiently large in the overdamped limit. Then the energy conversion rate at each time step can be definitely determined in terms of v_d as

$$d = d(v_d) = a_1 v_d + a_2 v_d^2, \quad (12)$$

yielding dynamic equations of the system as

$$\frac{de}{dt} = q(t) - ce - (a_1 v_d + a_2 v_d^2) e, \quad (13)$$

$$\gamma \frac{dx}{dt} = (a_1 + a_2 v_d) e + f_L + f_M + \zeta(t). \quad (14)$$

Equations (13) and (14) with the drift velocity in (11) define our modified energy depot model applicable to the overdamped system. We will analyze these equations in detail in the following section.

3 Simulation results

We perform the active Brownian dynamics simulation by adopting the system of a molecular motor. We set units of time, length, and energy as 30 ms, 8 nm, and $25k_B T$, respectively, and use dimensionless reduced units in the following discussions. We have simulated our modified model for various sets of a_1 and a_2 in order to find a suitable energy conversion function for the dynamics of processively walking motor. In this paper, we choose a particular set of values $a_1 = 10$ and $a_2 = 1$ that successfully reproduces the forward processive motion stepping 8 nm for 30 ms on average in the absence of an external load. To examine intrinsic properties of the model and identify a role of thermal noise, we perform simulations with and without thermal noise separately. Note that the energy supply as well as the modulation of the ratchet potential occurs stochastically regardless of thermal noise so that the dynamics of our model has a stochastic nature inherently even without thermal noise. Therefore, it is necessary to perform a long-time average to obtain physical quantities of the motor. We generate each stochastic trajectory for 10^9 time steps with the simulation time step $\Delta t = 10^{-4}$. λ is dependent upon ATP concentration C in a nonlinear manner. To find the relationship between λ and C , we use the well-known Michaelis–Menten (MM) relation. The MM relation was derived for enzyme kinetics and has been widely used, in particular, in analyzing a dependence of molecular motor activity on ATP concentration. Following the MM relation, we assume

$$\frac{1}{\lambda} = \frac{C}{C + C^*} \quad (15)$$

where C^* is the crossover concentration in the process of ATP delivery and hydrolysis. We use $C/C^* = 0.5, 1.0, 5.0$, and ∞ in our simulation, which corresponds to $\lambda = 3.0, 2.0, 1.2$, and 1.0 , respectively. In real dimensions, those correspond to 90, 60, 36, and 30 ms, respectively. For the other parameter values, we adopt the known biological ones for kinesin: $\gamma \sim 6$ pN·ms/nm, $U_{\text{strong}} = 9k_B T$ and $U_{\text{weak}} = k_B T$, $T = 300$ K, and the internal dissipation rate is chosen as $c = (6 \text{ ms})^{-1}$.

3.1 Without thermal noise

In this section, we present the simulation results in the absence of thermal noise. The average velocity as a function of the load, f_L , is shown in Fig. 1. Unless the magnitude of the load is sufficiently large, the average velocity does not change for a given ATP concentration, keeping the forward processivity. For sufficiently large loads, on the other hand, the average velocity decreases significantly as the load increases. The stall force at which the average velocity is zero is about 7.94 pN for the saturation concentration of ATP ($C/C^* = \infty$), which agrees with the known range of the stall force, 6–8 pN, of the kinesin system.

The plateau behavior of the average velocity can be accounted for as follows. By the load force whose magnitude is smaller than the stall force, the motor can hardly overcome the ratchet potential barrier in the backward direction. Then the forward active force dominates

Fig. 1 The average velocity vs. load force f_L in the absence of thermal noise for $C/C^* = \infty$, 5.0, 1.0, 0.5 where C is the ATP concentration and C^* the Michaelis–Menten constant. $C/C^* = \infty$ denotes the saturation concentration of ATP

so that the processive stepping occurs in synchronization with the random energy supply. As the magnitude of the load increases, the average velocity starts to decrease around $f_L = -U_{\text{strong}}/(2L/3) = -6.91$ pN at which the potential barrier in the backward direction disappears. For a load force comparable to the stall force, the particle drifts in the backward direction due to the load, with which the active force is balanced on average. For the loads exceeding the stall force, the motor will be detached in experiments, but it speeds up indefinitely in our model since the detachment mechanism is not included.

The effect of the ATP concentration shown in Fig. 1 can be understood as follows. When $f_L = 0$, the average velocity is expected to be proportional to λ^{-1} and follow the MM relation given by $v = \lambda^{-1} = C/(C + C^*)$, as observed in the previous studies. In contrast to those studies, however, our result shows that the stall force is dependent upon the ATP concentration. In the present model, the dynamics of a molecular motor is governed by the competition between the active force and the load, and their balance determines the stall condition. As the ATP concentration increases, the active force is generated more frequently and the magnitude of the stall force therefore should be larger.

For $C/C^* = \infty$ and $f_L = 0$, we obtain a trajectory during the elapsed time up to 10^5 time steps and measure the dwell time, whose distribution is shown in Fig. 2. There are only forward steps observed in this case, and the dwell time distribution follows the exponential distribution with a mean value comparable to unity. Therefore, one can conclude that the forward stepping occurs in synchronization with the stochastic energy supply, which is modeled to follow the exponential waiting time distribution. A part of the typical trajectory is depicted in the inset of Fig. 2. One can see that the average velocity is comparable to unity, and the trajectory is indeed a sequence of forward steps with variable dwell times.

At stall force, $f_L = -7.94$ pN, the dwell time distributions of the forward and backward steps for $C/C^* = \infty$ are shown in Fig. 3. It is found that the numbers of forward and backward steps are almost the same, yet their distributions are completely different. The results at the stall force can be understood as follows. If there were no energy supply, there would be no forward stepping and the dwell time of the backward movement would be around unity, since the backward drift due to the load occurs continuously with the average velocity around negative unity. On the other hand, when the stochastic energy is supplied, there occurs a competition between the forward active driving and the backward

Fig. 2 Dwell time distribution of the forward steps for $f_L = 0$ and $C/C^* = \infty$, the saturation concentration of ATP, in the absence of thermal noise. The *inset* shows a part of a typical trajectory

drift. The forward stepping is basically in synchronization with the stochastic energy supply. However, the forward stepping with a dwell time larger than unity is suppressed since the dwell time of the forward stepping is limited by that of the backward stepping. The dwell time distribution of the backward movement is centered around unity with a spread due to the stochastic forward stepping. Shown in the inset of Fig. 3 is a part of a typical trajectory at the stall force. The average velocity is approximately vanishing as expected and hence, the numbers of forward and backward steps are the same, as expected. It is worth mentioning that the active motor is in a dynamical equilibrium where the motor moves forward or backward with equal probability due to balancing between forward and backward driving forces, instead of being in an immobile state.

The numbers of forward and backward steps for $\lambda = 1$, or equivalently $C/C^* = \infty$, are counted and shown as a function of f_L in Fig. 4. When the load force is weak, the number of backward steps is vanishingly small and the trajectory mainly consists of forward steps as shown before. As the magnitude of the load force increases, the number of forward and

Fig. 3 Dwell time distributions of the forward (*solid line*) and backward (*dashed line*) steps at stall force ($f_L = -7.94$ pN) and $C/C^* = \infty$, the saturation concentration of ATP, in the absence of thermal noise. The *inset* shows a part of a typical trajectory

Fig. 4 Number of forward and backward steps vs. f_L for $C/C^* = \infty$ in the absence of thermal noise. The simulation is performed during 10^5 time steps, which correspond to the consumption of 10^5 ATP molecules on average. The motor goes one step forward for consumption of each ATP in stationary regime

backward steps decreases and increases, respectively. At the stall force, the numbers of forward and backward steps are the same and the motor ultimately diffuses around a fixed position.

3.2 With thermal noise

To examine an effect of thermal fluctuations, we performed the simulation by taking into account the Gaussian white noise as described above. The velocity as a function of f_L is plotted in Fig. 5 for various values of C/C^* . In contrast to the case without thermal noise, the velocity does not show a plateau behavior under assisting load force. This is the limitation of our model based on the Brownian dynamics, and there must be an additional apparatus to reproduce the plateau behavior such as consideration of the detachment rate of the motor. As the load increases, the velocity continuously decreases and vanishes around $f_L = -5.63$ pN for $C/C^* = \infty$, which is smaller in magnitude than the stall force in the absence of thermal noise. This implies that thermal noise enhances the probability of backward stepping in our model and hence the motor stalls at a relatively small load. The effect of thermal noise is

Fig. 5 The average velocity vs. load force f_L in the presence of thermal noise for $C/C^* = \infty$, 5.0, 1.0, 0.5 where C is the ATP concentration and C^* the Michaelis–Menten constant. $C/C^* = \infty$ denotes the saturation concentration of ATP

more pronounced when C/C^* is smaller, yielding a wider range of stall forces depending on the ATP concentration than that without thermal noise. The velocity is again inversely proportional to λ when $f_L = 0$ and follows the MM relation.

The dwell time distribution for $C/C^* = \infty$ and $f_L = 0$ is shown in Fig. 6. One can notice that the dwell time distribution of the forward stepping basically follows the exponential distribution of the energy input pulses as in Fig. 2. However, both forward and backward steps are enhanced significantly for short dwell times. This can be attributed to the effect of thermal fluctuations. Without thermal fluctuations, supply of a single energy pulse generates only a single forward step. The thermal fluctuations, however, cooperate with the energy pulses adjacent in time and can generate more forward steps than the number of supplied energy pulses. If an energy pulse is delivered to the motor immediately after the previous one, for instance, the two energy pulses can generate three or more forward steps. These cooperative effects occur only when the dwell time is smaller than $c^{-1} = 6$ ms, the internal relaxation time of the energy depot. The backward steps are not allowed without thermal fluctuations, as we have seen before. With the aid of thermal fluctuations, on the other hand, the thermal hopping could occur in a special situation. Since the barrier height of the ratchet potential is $9k_B T$, it is not probable to observe the thermal hopping when the particle is located around the potential minimum. However, immediately after a forward stepping, the particle may exist around the barrier top. Then the particle can re-cross the barrier due to thermal fluctuations, which is the reason why the backward movement occurs only with short dwell times. A part of a typical trajectory for $\lambda = 1$ and $f_L = 0$ is depicted in Fig. 6. One can observe that average velocity is comparable to unity again, yet the trajectory is a mixed sequence of forward and backward steps with variable dwell times. Regardless of thermal noise, our choice of the energy conversion function ($a_1 = 10$, $a_2 = 1$) yields the same average velocity for $C/C^* = \infty$ and $f_L = 0$.

At stall force, $f_L = -5.63$ pN for $C/C^* = \infty$ in the presence of the thermal noise, the dwell time distributions of the forward and backward steps are shown in Fig. 7. In contrast to the case without thermal noise, the distributions of the forward and backward steps are similar and basically behave exponentially. In this case, the barrier height is lowered from $U_{\text{strong}} = 9k_B T$ to $1.67k_B T$ due to the load force of $f_L = -5.63$ pN. Then the thermal fluctuations can generate backward hopping significantly, yielding an exponential distribution of dwell times. The average dwell time for the backward hopping is measured

Fig. 6 Dwell time distributions of the forward (solid line) and backward (dashed line) steps for $f_L = 0$ and $C/C^* = \infty$, the saturation concentration of ATP, in the presence of thermal noise. The inset shows a part of a typical trajectory

Fig. 7 Dwell time distributions of the forward (solid line) and backward (dashed line) steps at stall force ($f_L = -5.63$ pN) and $C/C^* = \infty$, the saturation concentration of ATP, in the presence of thermal noise. The inset shows a part of a typical trajectory

to be about 0.59 in reduced units. The forward stepping again should be in synchronization with the stochastic energy supply. However, the dwell time of the forward stepping is limited by the backward hopping and measured to be about 0.56, which is indeed shorter than 0.59. The enhancement of the forward and backward steppings with short dwell times is again due to the nonequilibrium effect as we have seen in the case of $f_L = 0$. Shown in the inset of Fig. 7 is a part of a typical trajectory at stall force. One can observe again the stall behavior as expected so that the average velocity is approximately vanishing and the numbers of forward and backward steps are the same as it should be. Note also that the fluctuations in the trajectory are larger than those for $f_L = 0$.

The numbers of forward and backward steps for $C/C^* = \infty$ are counted and plotted as a function of the load force in Fig. 8. It is interesting to see that both the numbers of forward and backward steps are increased compared to the case without thermal noise. Note also that the number of backward steps is nonzero finite even when $f_L = 0$. Moreover, a significant enhancement of the backward stepping with increasing load strengths yields the smaller stall force in comparison to the case without thermal noise.

Fig. 8 Number of forward and backward steps vs. f_L for $C/C^* = \infty$ in the presence of thermal noise. The simulation is performed during 10^5 time steps, which correspond to the consumption of 10^5 ATP molecules on average. The motor goes one step forward for consumption of each ATP in stationary regime

4 Concluding remarks

We have presented a modified active Brownian dynamics model. By considering the simplest asymmetric energy conversion rate function, we revisited our generalized energy depot model and found that the active mechanism becomes more effective due to the asymmetry when the model is applied to a processive molecular motor system. With the asymmetry, the model depicts a genuine stepping dynamics which is not possible with the symmetric model. By introducing stochastic energy supply, flashing ratchet potential synchronized with the energy supply, and thermal noise, we applied our model to a system of a processive motor on a microtubule.

The average velocity is obtained as a function of the load force for different energy-supply rates, which are related to ATP concentrations via the Michaelis–Menten relation. In the absence of thermal noise, the stall force at which forward and backward stepping motions are equally probable ranges in the well-known values of 6–8 pN and our active motor can keep the average velocity even under few pN assisting load as observed in the conventional kinesin. However, if thermal noise is turned on, then the stall force gets smaller in magnitude and our motor speeds up slowly without saturation as the assisting load increases. We expect that the present model has to include some other ingredient such as a detachment mechanism to fix these discrepancies to kinesin. The stall force in our model turned out to be ATP-dependent, regardless of thermal noise, in contrast to kinesin. This might be the limitation of the simple mapping of the energy-supply rate to the ATP concentration via the Michaelis–Menten relation. Still, the detailed statistical analysis on trajectories will be useful in understanding a rough mechanism of the processive motor dynamics. The numbers of forward and backward steps were counted and the dwell time distributions for various cases were obtained. An effect of thermal fluctuations was found to be crucial in the dynamics of the active particle.

We would like to emphasize that our modified energy depot model is able to describe an overdamped active Brownian dynamics in the presence of thermal noise. A standard energy depot model cannot describe properly the dynamics of the overdamped particle as long as an energy conversion rate function depends on its velocity, since the velocity is not well-defined. Our present model overcomes this difficulty by introducing a well-defined drift velocity. This approach extends, in general, applicability of the energy depot model to a wide variety of situations where thermal fluctuations are important.

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