2012 American Control Conference
Fairmont Queen Elizabeth, Montréal, Canada
June 27-June 29, 2012

Maximizing Transport in Open Loop for Flashing Ratchets

Subhrajit Rowchowdhury, Srinivasa Salapaka, Murti Salapaka

***Abstract*— This paper studies open-loop operation of *flashing ratchets*, which refer to mechanisms that enable motion of particles under diffusion and possibly drag forces along a preferred direction through alternating turning on and off of specifically designed *ratchet* potentials. Flashing ratchets are used to model certain transport mechanisms of molecular motors and are of special interest to biologists and biophysicists. Mathematically they are are modeled by stochastic hybrid systems. For an open-loop design of *on-times* and *off-times*, we derive, under certain practical assumptions, an exact probability density function that reflects the spatial distribution of particles in space after the ratchet has flashed a given number of times, and find an *optimal off-time* that maximizes the transport velocity for a specific ratchet potential. Validation of the underlying assumptions is also presented. Simulation results show that these open-loop designs achieve as good or better average velocities for particles over certain well known existing feedback strategies in literature.**

I. Introduction

Thermal noise, in general, is viewed as having a detrimental effect on the system performance. Feynman, however, pointed out in [8] that Brownian motion can be used to achieve a non-zero mean displacement using ratchet-pawl principle[1], and hence, useful work can be extracted from non-equilibrium microscopic sources (*e.g.,* chemical potentials) using thermal noise, if an appropriate thermal gradient is maintained[2]. Recently, using the same principle, it has been shown that using a ratchet-shaped periodic potential, that switches on and off alternatingly [3] (and hence the name *flashing ratchet*), or switches between two different potential levels [2], transportation against a load force can be achieved for nano-machines. Later, [9], [14] has shown that the potential need not be necessarily a ratchet shaped one; any periodic potential with a broken symmetry would serve the purpose. Also, it has been shown that the switching between two levels (or on and off) can be deterministic as well random in nature [10]. In this paper, we focus on the flashing ratchet system with deterministic switching times. Besides physicists and engineers, the flashing ratchet model is also of special interest to biologists and biophysicists who study the transport mechanisms of molecular motors, as certain theories are postulated that connect the two ([1], [2], [4], [11], [13]). Thus, a deeper understanding of this mechanism and development of new theories will help a diverse scientific community.

Subhrajit Rowchowdhury is with Electrical and Computer Engineering Department at University of Minnesota, Twin Cities subhra@umn.edu
Srinivasa Salapaka is with Faculty of Mechanical Engineering, University of Illinois at Urbana Champaign salapaka@illinois.edu
Murti Salapaka is with Faculty of Electrical and Computer Engineering Department at University of Minnesota, Twin Cities murtis@umn.edu

[1]Hence the name *Brownian ratchet*

[2]Note that, thermal noise is used to extract work from other sources and not from itself, and thus the methodology does not violate the laws of thermodynamics.

The basic principle of particle transport in flashing ratchet systems is discussed extensively in [3], [9], [12], [14]. The equation of motion of a particle in a flashing potential field with an external load force F can be written as

$$m\ddot{x}(t) = -\Theta(t)V'(x(t)) - \gamma\dot{x}(t) - F + \xi(t) \qquad (1)$$

where m is the mass of the particle, $V(x)$ is a spatially periodic potential with period L that satisfies $V(x) = V(x+L)$, γ is the drag coefficient of the medium and $\xi(t)$ represents thermal noise with $<\xi(t)>=0$ and $<\xi(r)\xi(s)>=2\gamma k_B T\delta(r-s)$, where k_B denotes the Boltzmann's constant and T the absolute temperature, and $x(t)$ represents a sample realization of the random process. Here, $\Theta(t)$ is a dichotomous switching function defined as

$$\theta(t) = \begin{cases} 1 \text{ for } t \bmod T \in [0, T_{on}) \\ 0 \text{ for } t \bmod T \in [T_{on}, T_{on}+T_{off}) \end{cases} \qquad (2)$$

where T_{on} and T_{off} are the on-time and off-time, the flashing period being $T = T_{on} + T_{off}$.

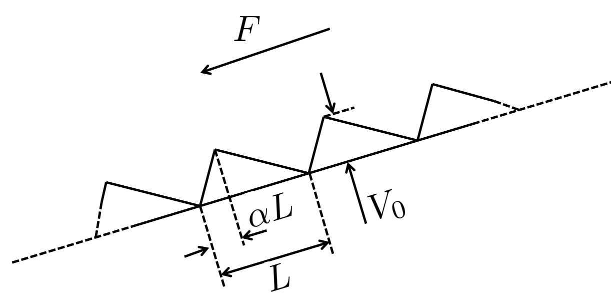

Fig. 1. The ratchet potential is described here. V_0 denotes the height of the potential barrier and typically $V_0 >> k_B T$, where k_B denotes the Boltzmann's constant and T the absolute temperature. L denotes the spatial period of the potential and α decides how steep the potential barrier is. Typically $\alpha << 0.1$. F denotes the load force on the particle.

We take the potential function $V(x)$ to be as follows ([5]):

$$V(x) = \begin{cases} V_0 \dfrac{x}{\alpha L} \text{ for } x \bmod L \in [0, \alpha L) \\ V_0 \left(1 - \frac{1}{1-\alpha}\left(\frac{x}{L} - \alpha\right)\right) \text{ for } x \bmod L \in [\alpha L, L) \end{cases} \qquad (3)$$

where V_0 denotes the height of the potential barrier, typically taken to be several times of $k_B T$, and the parameter α decides the slope of the potential function. Note that, a key property of the spatially periodic potential is its *broken symmetry*, *i.e.*, there does not exist any Δx such that $V(-x) = V(x + \Delta x)$, for all x (see Fig. 1)without which no net uphill transport will occur([3], [9], [12], [14]).

To facilitate transport, the choice of T_{off} should be such that the particles residing at any valley have enough time to diffuse to the next valley through the potential barrier crossing the distance αL when the potential is off. However T_{off} should be small enough so that particles do not diffuse backwards to the previous valley crossing the distance $1 - \alpha L$. From these considerations, T_{off} is typically chosen to be $\frac{(\alpha L)^2}{2D}$[3]([12]). The choice of T_{on} should ensure localization of the particles trapped in a valley at its lowest point when the potential is on. Again, too high a value of on-time is not recommended as that will require more energy input and also slow down the transport velocity by increasing the flashing period. This requires $T_{on} = \dfrac{\gamma(1-\alpha)L}{\frac{V_0}{(1-\alpha)L} + F}$. The detailed derivation of on-time and off-time can be found in [3], [12].

An important use of flashing ratchets in engineering systems is in separation of particles in a mixture. [3] discusses about an apparatus for such purpose where using appropriate external modulation, particles of slightly different sizes can be made to move in different directions by exploiting the fact that due to their difference in size, they will experience different level of friction and Brownian motion. To speed up the separation process, the relative velocity between the two types of particles has to be increased, which can be achieved by increasing the transport velocities of the different particles to different extents. Closed-loop techniques ([5], [6]) have been applied to increase the transport velocity, but the huge number of particles involved in separation processes render these techniques unusable from hardware requirement point of view, as we need sensors to monitor the position of each particle at every sampling instant. In this paper, we present a way to maximize the transport velocity in open-loop that requires no extra hardware or real time processing, but the velocity achieved is shown to be comparable or better than reported closed-loop methods for high number of particles.

This paper is organized as follows: In Sec. II we formulate the problem of obtaining an exact pdf of the distribution of particles after a certain number of flashes by writing a master equation. In Sec. III, under certain assumptions we derive a pdf and check the validity of our assumptions by calculating error bounds. We also state a few results that give us estimates of stalling force and maximum allowable on-time and off-time for non-zero load force, and error bounds arising from the estimates. Then in Sec. IV from the pdf we analytically calculate the steady state average transport velocity and its variance, and then from that we calculate the *optimal off-time* that will maximize the open-loop transport velocity. Finally, in Sec. V through simulations we show that the open-loop velocity obtained by calculating *optimal off-time* is similar or better than the velocity obtained by closed-loop methods ([5], [6]) for high number of particles. Thus, in situations where applying feedback might not be realistic due to high number of particles involved, our method proves to be better as it does not require any additional hardware. Further insights and discussions about our strategy and its practical applicability is discussed in Sec. VI.

[3]Strictly speaking, this should be chosen to be the off-time for zero load force. Following the same logic, for load force F, T_{off} should be chosen to be the non-extraneous solution of the quadratic equation $(\alpha L + T_{off}\frac{F}{\gamma})^2 = 2DT_off$. Here D is the diffusion constant defined later in (6).

II. Problem Formulation

Consider a particle to be initially located at valley 0 (see Fig. 2). The valleys to the left of valley 0 are numbered as -1, -2, $\ldots$, $-j$ and so on. Similarly, to the right they are numbered as 1, 2, $\ldots$, i and so on. The probability of jumping forward by i valleys in a single flash is denoted by s_i and that of jumping backward by j valleys is denoted by s_{-j} for the particles.

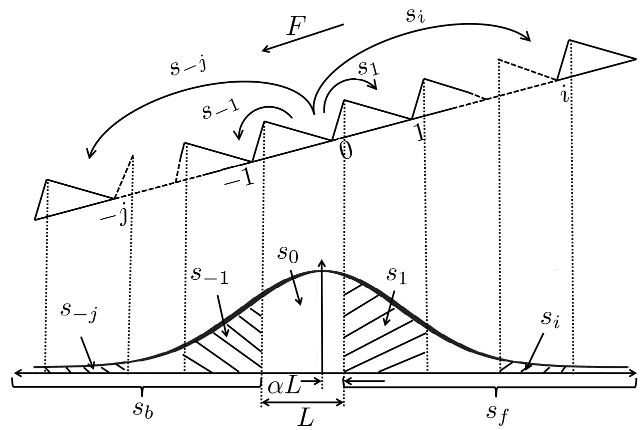

Fig. 2. Flashing ratchet showing the numbering of valleys and different transition probabilities. The valley where the particle(s) initially reside is marked as the zeroth valley. Valleys towards its right are numbered with positive integers and to the left with negative ones. The probability of jumping forward by i valleys is denoted by s_i, whereas that of jumping backwards by j valleys is denoted by s_{-j}. s_0 denotes the probability of remaining in the initial valley, while s_f and s_b denote the total probability of transportation to the front and to the back respectively.

Under the assumption of overdamped condition([9], [12], [14]), the equation of motion (1) becomes,

$$\gamma \dot{x}(t) = -V'(x(t)) - F + \xi(t). \tag{4}$$

If the particle is at the bottom of the zeroth valley at $t = 0$ and the ratchet potential is turned off, then the corresponding distribution of the position of the particle $x(T_{off})$ at the end of off-time becomes

$$p(x(T_{off}), T_{off}|0,0) = \frac{exp\left(-\frac{(x+\frac{F}{\gamma}T_{off})^2}{4DT_{off}}\right)}{\sqrt{4DT_{off}}}, \tag{5}$$

where the diffusion constant D is given by the Einstein's relation [12]

$$D = \frac{k_B T}{\gamma}. \tag{6}$$

If we assume that the on-time T_{on} is long enough to to drive the particle to the bottom of its resident valley[4], then by the same argument for each flash, it can be shown that

$$s_i = P(il + \alpha L \leq x(T_{off}) \leq (i+1)L + \alpha L)$$

and

$$s_{-i} = P(-(i+1)L-(1-\alpha)L \leq x(T_{off}) \leq -iL-(1-\alpha)L)$$

where $P(a \leq x \leq b) = \int_a^b p(x(T_{off}), T_{off}|0,0)dx$. Here, during the on-time, we have neglected the particle displacements due to diffusion compared to those due to the applied ratchet potential.

We also define the quantities $s_b = \sum_{j=1}^{\infty} s_{-j}$, $s_f = \sum_{i=1}^{\infty} s_i$, and $s_0 = 1 - s_f - s_b$, where s_f and s_b denote the total probability of transportation to the front and to the back in a single flash respectively and s_0 denotes the probability of remaining in the initial valley.

The probability $P_k[n]$ of finding the particle in the k^{th} valley after the n^{th} flash is given by

$$P_k[n] = P_k[n-1]s_0 + \sum_{i=1}^{\infty} P_{k+i}[n-1]s_{-i} + \sum_{i=1}^{\infty} P_{k-i}[n-1]s_i, \tag{7}$$

where the first term in (7) signifies the probability of the particle that remain in the k^{th} valley, the second term represents the probability of the particle coming into the k^{th} valley from valleys in front and the third term represents the probability of the particle coming into the k^{th} valley from the valleys behind in the n^{th} flash. As $P_k[0] = \delta[k]$ for all k, it follows that if we can determine s_i and s_{-i} for all i, then we can determine the probability distribution of the particles in space after any number of flash by propagating (7).

III. Derivation of PDF

Although it is possible to derive the pdf for position of the particle (which valley it belongs) by propagating (7) for a given initial condition, it is desirable from analytical and practical considerations to bound the position jump in a single flash to a finite number of valleys. To obtain such a bound, we first study the necessary conditions on physical parameters such as load force and off time that ensure preferential (forward) transport. In this section, we state two theorems that give us the limit on load force and upper and lower bounds on off-time, beyond which negligibly small forward transport occurs. Following that, we present theorems that quantify bounds on backward propagation beyond a certain valley for the load force and off-time parameters that ensure sufficiently large forward propagation. From these theorems, we truncate the extent of jumps in a single flash to only adjacent valleys ([3]), or even totally neglect the backward propagation ([12]) and derive closed form pdf for the particle propagation. We show that the error introduced by approximating bi-infinite number of valleys by just the adjacent valleys or even totally neglecting back propagation is less than 0.1% for appropriately chosen off-time.

[4]Higher values of V_0 and lower values of α and L, i.e., valleys with a steeper shape, will also help hold this assumption good.

A. Ensuring Forward Transport

Theorem 1: Let $F_{stall} = \dfrac{\gamma n^2 D}{2\alpha L}$. If load force $F > F_{stall}$, then $\sum_{i>0} s_i \leq \frac{1}{2}\text{erfc}(\frac{n}{\sqrt{2}})$ for any choice of off-time, where $\text{erfc}(x) = \frac{2}{\sqrt{\pi}} \int_x^{\infty} e^{-y^2} dy$.

Proof: Left to reader.

This theorem essentially gives an estimate for the *stalling force*. In physical systems that mimic this mechanism, such as molecular motor transport ([4], [11], [2], [12]), stalling force is defined as the minimum value of load force beyond which no forward transport occurs for any choice of on-time and off-time. For $n \geq 3$, $\frac{1}{2}\text{erfc}(\frac{n}{\sqrt{2}}) \leq 0.00134989803$. Thus, by choosing $n \geq 3$, we can obtain a practical estimate for the stalling force.

Theorem 2: Let load force $F < F_{stall}$ and off-time $T_{off} \notin (T_l, T_u)$, where

$$T_l = \left(\frac{\sqrt{2Dn^2} - \sqrt{2Dn^2 - \frac{4\alpha LF}{\gamma}}}{2\frac{F}{\gamma}} \right)^2$$

and

$$T_u = \left(\frac{\sqrt{2Dn^2} + \sqrt{2Dn^2 - \frac{4\alpha LF}{\gamma}}}{2\frac{F}{\gamma}} \right)^2.$$

Then $\sum_{i>0} s_i \leq \frac{1}{2}\text{erfc}(\frac{n}{\sqrt{2}})$, where $\text{erfc}(x) = \frac{2}{\sqrt{\pi}} \int_x^{\infty} e^{-y^2} dy$.

Proof: Left to reader.

Corollary 3: If load force $F < F_{stall}$ and off-time $T_{off} \in (T_l, \hat{T}_{off})$, where $\hat{T}_{off} = \dfrac{\alpha L}{\frac{F}{\gamma}}$, then $\sum_{i>0} s_i > \frac{1}{2}\text{erfc}(\frac{p}{\sqrt{2}})$ for all $p > 3$. We call this condition to be *non-negligible forward transport*.

Proof: Left to reader.

This theorem together with the corollary gives us upper and lower bounds on off-time to ensure non-negligible forward transport. The lower bound is explained since the probability of the particle diffusing to the next valley is small when the off time T_{off} is small. The higher bound exists since a sufficiently large T_{off} will make the the downhill drift term $\frac{F}{\gamma}T_{off}$ large enough to overwhelm the diffusion term that causes the forward transport. In either case, forward transport will be negligible.

B. Bounding Backward Propagation

Theorem 4: If $F \in (F_m, F_{stall})$, where $F_m = \dfrac{2n^2 D\gamma\alpha}{(m+1-2\alpha)^2 L}$, and we ensure non-negligible forward transport, by $\sum_{i>0} s_i > \frac{1}{2}\text{erfc}(\frac{p}{\sqrt{2}})$ for all $p > 3$, by selecting off-time t such that $t \in [T_l, \hat{T}_{off}]$, then $\sum_{i<-m} s_i \leq \frac{1}{2}\text{erfc}(\frac{n}{\sqrt{2}})$, where $\text{erfc}(x) = \frac{2}{\sqrt{\pi}}\int_x^\infty e^{-y^2}dy.$

Proof: Left to reader.

This theorem states that if the load force is greater than a certain value, but less than the stalling force, then under the conditions that non-negligible forward transport is occurring, backward propagation beyond a certain valley can be neglected. This might seem non-intuitive at first glance, as increasing load force is supposed to increase back propagation. The key thing to note here is, we are only interested in cases where a non-negligible forward transport takes place. A non-negligible forward transport is ensured in the form of $\hat{T}_{off}$, a maximum limit on the off-time. We can see that $\hat{T}_{off}$, and hence the maximum variance $2D\hat{T}_{off}$ is a decreasing function of load force. Thus, with increase in load force, the distribution of particles about its mean during the off-time becomes sharper, and hence back propagation beyond a certain valley can be neglected.

Theorem 5: Let $F \in (0, F_{stall})$ and $T_{off} < min(T_m, \hat{T}_{off})$, where

$$T_m = \left(\frac{-\sqrt{2Dn^2} + \sqrt{2Dn^2 + \frac{4(m+1-\alpha)LF}{\gamma}}}{2\frac{F}{\gamma}}\right)^2$$

If non-negligible forward transport is ensured by $\sum_{i>0} s_i > \frac{1}{2}\text{erfc}(\frac{p}{\sqrt{2}})$ for all $p > 3$, then $\sum_{i<-m} s_i \leq \frac{1}{2}\text{erfc}(\frac{n}{\sqrt{2}})$, where $\text{erfc}(x) = \frac{2}{\sqrt{\pi}}\int_x^\infty e^{-y^2}dy$. If $F = 0$, similar condition holds for

$$T_m = \frac{(m+1-\alpha)L}{\sqrt{2Dn^2}}$$

Proof: Left to reader.

This theorem gives us a way to limit back propagation beyond a certain valley by controlling the off-time if the condition in Theorem 4 is not met. The condition $T_{off} < min(T_m, \hat{T}_{off})$ ensures non-negligible forward transport in case $T_m > \hat{T}_{off}$.

C. Derivation of pdf

If the physical parameters and choice of off-time allow us to keep back propagation beyond the adjacent valley negligible, which is true for many physical cases([3]), then we may re-define the following quantities as follows:

- $s_f = s_1 \equiv$ probability of jumping one valley forward
- $s_b = s'_{-1} \equiv$ probability of jumping one valley backward
- $s_0 = 1 - s_f - s_b \equiv$ probability of staying in the same valley

From (7), the propagation equation becomes

$$P_k[n] = s_0 P_k[n-1] + s_b P_{k+1}[n-1] + s_f P_{k-1}[n-1] \quad (8)$$

Taking $\mathfrak{Z}$ transform over space, we obtain,

$$P_z[n] = s_0 P_z[n-1] + z s_b P_z[n-1] + z^{-1} s_f P_z[n-1] \quad (9)$$

which implies that

$$P_z[n] = (s_0 + z s_b + z^{-1} s_f)^n P_z[0] \quad (10)$$

Now, suppose the particle was initially assumed to be in the zeroth well, *i.e.*, $P_k[0] = \delta[k]$. Thus $P_z[0] = 1$. It follows that,

$$P_z[n] = (s_0 + z s_b + z^{-1} s_f)^n \quad (11)$$

Expanding the trinomial and collecting similar terms, we can write the coefficient of z^{-i} in the expansion to be $\sum_{\substack{p,q,r\geq 0\\ p+q+r=n\\ r-q=i}} \binom{n}{p,q,r} s_0^p s_b^q s_f^r$, where $i \in \mathcal{Z} \cap [-n, n]$.

Noting that, $\mathfrak{Z}^{-1}[z^{-i}] = \delta[k-i]$ for all $i \in \mathcal{Z}$, inverse $\mathfrak{Z}$ transform of the expansion of (11) gives us,

$$P_k[n] = \sum_{\substack{p,q,r\geq 0\\ p+q+r=n\\ r-q=k}} \binom{n}{p,q,r} s_0^p s_b^q s_f^r \quad (12)$$

where $k \in \mathcal{Z} \cap [-n, n]$.

Motivated from conditions in Theorems 4 and 5, if we put $s_b = 0$ in (11),*i.e.,* we neglect back propagation as well ([12]), we get ,

$$P_z[n] = (s_0 + z^{-1} s_f)^n \quad (13)$$

Applying the initial condition $P_z[0] = 1$ and taking inverse $\mathfrak{Z}$ transform, in this case we obtain,

$$P_k[n] = \binom{n}{k} s^k (1-s)^{n-k} \quad (14)$$

where $s_f = s$ and hence $s_0 = 1 - s$.

The *optimal off-time*, the off-time that optimizes the average transport velocity (determined in the next section), satisfies the assumptions in Theorems 1-5 and hence (14) becomes the constitutive equation. However certain designs may solicit the use of (12).

IV. Derivation of Average Velocity and Optimal Off-Time

In this section, we derive the expression for steady state average velocity of a particle under a flashing ratchet potential. It becomes evident from this expression that maximizing the probability of forward jump (i.e., maximizing s) does not necessarily increase the transport velocity, which is a nonlinear function of off-time, for fixed values of all other physical parameters. Since, the design of on-time is done to ensure that the particle is driven to the bottom of valley before the potential flashes off ([3], [12]), it does not have significant effect on the average velocity. Also, in practice the physical parameters are not alterable and therefore do not constitute control parameters. Hence, the only parameter that gives us control over the average velocity is the off-time, and we derive an off-time that maximizes the transport velocity. We show that in the long time limit, the variance of the average velocity becomes zero, thus giving us a high confidence in our calculated steady state average velocity. It is to be noted that although we have derived the p.d.f. for one particle, it is equivalent to the spatial distribution for a large number of identical particles, provided identical forces act upon them and they do not have any coupling among each other. Thus, the different physical quantities calculated for a single particle applies to the respective quantities of the center of mass of an ensemble of particles.

A. Average Velocity and Variance

From (14), the expected position of a particle after n^{th} flash is given by

$$< x_n > = L \sum_{k=0}^{n} k P_k[n] = nLs$$

Thus, the average velocity is given by

$$< v_n > = < v > = \frac{nLs}{n(T_{on} + T_{off})} = \frac{Ls}{T_{on} + T_{off}} \quad (15)$$

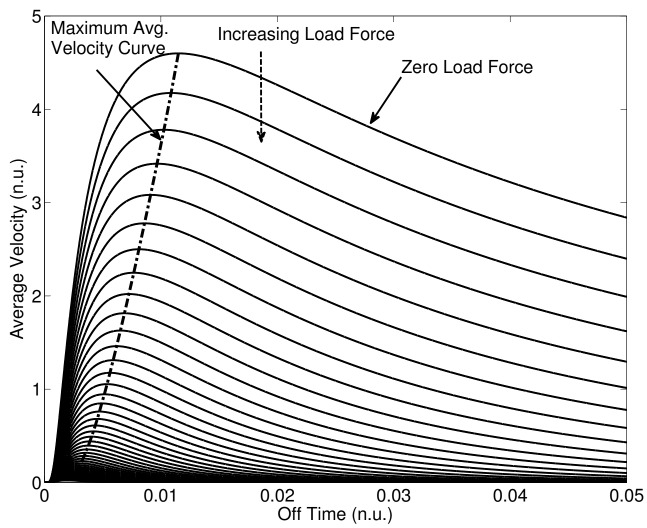

Fig. 3. The variation of average velocity with off-time for different load forces is shown above. T_{on} is taken to be $\frac{\gamma(1-\alpha)L}{\frac{V_0}{(1-\alpha)L}+F}$ and other physical parameters are chosen as $\alpha = 0.1$, $V_0 = 50k_BT$, $\gamma = 1$ and $L = 1$. All units are normalized (n.u.) in terms of γ and L. It can be clearly seen that for each load force, the average velocity achieves a maximum for a particular off-time, which we term as the *Optimal Off-Time*.

This expression is in agreement with what [12] derives based on intuitive arguments. Thus we can see that the average velocity remains constant and hence independent on the number of flashes. We also note that, as s is a function of T_{off}, so is the average velocity. Fig. 3 shows the variation of average velocity with off-time for different load forces and for a fixed set of physical parameters. As expected, the maximum velocity decreases with load force. This way, for a specific set of physical parameters, we can estimate the stalling force as well.

From (14), the second moment $< x_n^2 >$ of the position of the particle is given by

$$< x_n^2 > = L^2 \sum_{k=0}^{n} k^2 P_k[n] = n(n-1)L^2 s^2 + nL^2 s.$$

Therefore

$$< v_n^2 > = < v_n >^2 - \frac{L^2 s^2}{n(T_{on} + T_{off})^2} + \frac{L^2 s}{n(T_{on} + T_{off})^2}$$

Hence, the variance Δv_n^2 in the velocity of the particle is given by

$$\begin{aligned} < \Delta v_n^2 > &= < v_n^2 > - < v_n >^2 \\ &= \frac{L^2 s}{n(T_{on} + T_{off})^2}(1 - s) \end{aligned}$$

Thus, in the long time limit, we have,

$$< \Delta v_\infty^2 > = < \Delta v^2 > = 0$$

B. Optimal Off-Time

The expression of average velocity in (15) can be written as

$$< v > = \frac{Ls}{T_{on} + T_{off}} = \frac{erfc(\frac{\alpha L - \frac{F}{\gamma} T_{off}}{\sqrt{4DT_{off}}})L}{2(T_{on} + T_{off})} = f(T_{off}) \quad (16)$$

From Fig. 3 we note that for a given load force, the average velocity achieves a maximum for a particular T_{off}. The analytical way to find it would be to set the derivative of $f(T_{off})$ to zero and solve for T_{off}. We call this the *optimal off-time* for the given load force and set of physical parameters.It can be easily checked that this *optimal off-time* lies within the bounds described in Theorem 5 and thus the assumption of no back propagation holds good.

V. Simulation results

In this section we substantiate the advantage of calculating the *optimal off-time* to achieve maximum transport in open loop for high number of particles. To this end, we compare the transport velocity obtained by optimal T_{off} calculation with that obtained by the closed-loop method described in [5], [6] for different number of particles and for a specific set of physical parameters through Monte Carlo simulations on actual physical models[5]. From Fig. 4, we can also see that the velocity obtained from simulation closely matches to the velocity obtained from the theoretical calculations. Also, we can see that for high number of particles, the open loop method performs as good or better than the closed-loop method described in [5], [6].

This is because the performance of the closed-loop method depends on the change of the direction of net force acting on the particle ensemble, which essentially generates the control

[5]which are conducive to perfect localization, but we do not assume discrete flashes. Rather, we use the original dynamics in continuous time.

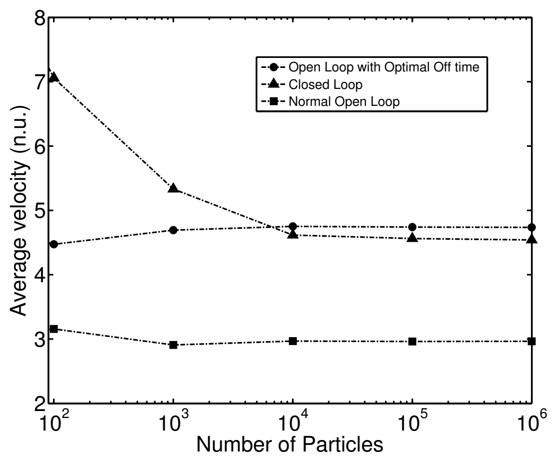

Fig. 4. The performances of the three methods, namely, the closed-loop method [5], [6], the normal open-loop method with $T_{off} = \frac{(\alpha L)^2}{2D}$ and our open-loop method with optimal T_{off} are compared in terms of average velocity achieved for no load force. T_{on} is taken to be $\frac{\gamma((1-\alpha)L)^2}{V_0}$ in all the three cases. The physical parameters are chosen as $\alpha = 0.1$, $V_0 = 50k_BT$, $\gamma = 1$ and $L = 1$. All units are normalized (n.u.) in terms of γ and L. It is apparent that our method performs as good as or better than the closed-loop method for high number of particles and considerably outperforms the normal open-loop method.

effort for the system. For high number of particles, due to Gaussian distribution of particles, the net force is always close to zero, thereby considerably bringing down the control effort. This explains why the the velocity for the closed-loop method sharply decreases with the increase in particle number. Also, the closed-loop method requires sensing the position of every particle at each sampling instant, which might not be very practical for very high number of particles.

The *optimal off-time* calculation method, however, does not depend on the number of particles. In fact, as it is a strategy based on probabilistic calculation, higher number of particles should favor it (which can be observed in Fig. 4). Essentially, the velocity obtained by this method remains more or less constant over the variation of number of particles. Also, as no decision has to be made in real time during operation, we can dispense of with sensors and the associated loop delays (see [7]) in this case. Thus, it performs better on both counts. Also, as expected, it can be seen that our optimal off time calculation method performs better than other open-loop methods having different formulas for off-time calculation reported in [3], [12].

VI. Conclusion and Discussions

In this article we have discretized the deterministic flashing ratchet model in time under mild assumptions. By discretization in time we mean that in the derivations we neglect any dynamics during on-time, *i.e.*, we assume the process to be consisting of discrete flashes. That way we were able to have many physical insights about the system and the model becomes much more mathematically tractable. This way, we derived the closed form p.d.f. of particle distribution after arbitrary number of flashes which in turn was used to obtain closed form expression for important quantities like steady state average velocity, mean square position and variance of velocity. We also discussed why such assumptions should be valid. We showed that in long term limit the variance of velocity goes to zero, which indicates that we will have high confidence in our calculated value of steady state average velocity. Hence, through Monte Carlo simulations on a physical model, we were able to show that the derived velocity matches closely with that obtained from simulation results in actual physical models.

One important advantage of obtaining a closed form p.d.f. and from there an expression of average velocity[6] was to be able to find an optimal off-time. The theorems in Sec. III-A and Sec. III-B together with the strategy in Sec. IV-B gives us a systematic way to design the off-time that would maximize velocity in open-loop for a given load force and given set of physical parameters. This velocity was shown to be considerably greater than achieved by not so rigorous off-time calculation methods described in [12]. Also, for high number of particles, the method performs similarly or better than closed-loop methods reported in [5], [6] without even encountering the loop delay problems mentioned in [7]. Due to this reason, this strategy is more suitable for applications where high number of particles are involved, e.g., the mixture separation apparatus discussed in [3].

References

[1] Rachid Ait-Haddou and Walter Herzog. Brownian ratchet models of molecular motors. *Cell Biochemistry and Biophysics*, 38:191–213, 2003. 10.1385/CBB:38:2:191.

[2] R. Dean Astumian and Martin Bier. Fluctuation driven ratchets: Molecular motors. *Phys. Rev. Lett.*, 72:1766–1769, Mar 1994.

[3] R.D. Astumian. Thermodynamics and kinetics of a brownian motor. *Science*, 276(5314):917, 1997.

[4] Martin Bier. The stepping motor protein as a feedback control ratchet. *Biosystems*, 88(3):301 – 307, 2007. BIOCOMP 2005: Selected papers presented at the International Conference - Diffusion Processes in Neurobiology and Subcellular Biology, BIOCOMP2006: Diffusion Processes in Neurobiology and Subcellular Biology.

[5] F. J. Cao, L. Dinis, and J. M. R. Parrondo. Feedback control in a collective flashing ratchet. *PHYS.REV.LETT.*, 93:040603, 2004.

[6] E.M. Craig, N.J. Kuwada, B.J. Lopez, and H. Linke. Feedback control in flashing ratchets. *Annalen der Physik*, 17(2-3):115–129, 2008.

[7] M. Feito and F. J. Cao. Time-delayed feedback control of a flashing ratchet. *Phys. Rev. E*, 76:061113, Dec 2007.

[8] R.P. Feynman, R.B. Leighton, M. Sands, et al. *The Feynman lectures on physics*, volume 2. Addison-Wesley Reading, MA, 1964.

[9] P. Hanggi, F. Marchesoni, and F. Nori. Brownian motors. *Annalen der Physik*, 14:5170, 2005.

[10] J. Kula, M. Kostur, and J. Luczka. Brownian transport controlled by dichotomic and thermal fluctuations1. *Chemical physics*, 235(1-3):27–37, 1998.

[11] D. Lacoste and K. Mallick. Fluctuation theorem for the flashing ratchet model of molecular motors. *Phys. Rev. E*, 80:021923, Aug 2009.

[12] H. Linke, M.T. Downton, and M.J. Zuckermann. Performance characteristics of brownian motors. *Chaos*, 15(2):26111, 2005.

[13] Katsuhiro Nishinari, Yasushi Okada, Andreas Schadschneider, and Debashish Chowdhury. Intracellular transport of single-headed molecular motors kif1a. *Phys. Rev. Lett.*, 95:118101, Sep 2005.

[14] P. Reimann and P. Hanggi. Introduction to the physics of brownian motors. *Applied Physics A: Materials Science and Processing*, 75:169–178, 2002. 10.1007/s003390201331.

[6]which is same as that stated intuitively without any rigorous explanation in [12]