Optimal switching time in Brownian Motors

Peter Thill
MIT Department of Chemistry
(Dated: May 16, 2013)

Here we study how the optimal switching time for a ratchet potential in a Brownian motor varies as a function of the potential's parameters. Though there are several papers which look at the efficiency of the motor in a more precise thermodynamic sense as a gauge of 'optimality'[1][2], we study the problem here in a much simpler context. We will simply define optimality as the quickest means of transporting the particle N 'steps' along the asymmetric potential. We show that the optimal time can have two different scalings with the depth of the potential well depending on model parameters. We study the effects of dimensionality on optimal switching time and also investigate how promoting switching parameters to random variables changes the distribution of threshold crossing times.

I. INTEGRATION SCHEME

We begin by studying the 1D Brownian motor. We will consider the particle to be infinitely damped such that the Langevin equation governing its motion is given by

$$\begin{aligned} \dot{x} &= -\frac{\mathrm{d}U}{\mathrm{d}x} + \eta(t) \\ \langle \eta(t)\eta(t')\rangle &= 2d\delta(t-t') \end{aligned} \tag{1}$$

In determining our choice of potential, we will have to be sensitive to the integration scheme used. Such Langevin equations are typically integrated using an Euler scheme:

$$\begin{aligned} \mathrm{d}x &= -v(x)\delta t + \left(\sqrt{2d\delta t}\right)\eta \\ v(x) &= \left.\frac{\mathrm{d}U(x')}{\mathrm{d}x'}\right|_{x'=x},\ \eta \sim \mathcal{N}(0,1) \end{aligned} \tag{2}$$

As such, we cannot use the sawtooth potential since it discontinuously jumps, and this will lead to unphysical numerical results as the particle can hop across the barrier even if it does not have adequate thermal energy. To remedy this, the asymmetric potential we will consider will be decaying linearly to its minimum point beyond which there will be a quadratic potential exerting a restoring force to the minimum. The free parameters we need to describe the potential are then the depth of the well, the slope of the linear portion, and the distance over which the quadratic potential rises back to the height of the potential well. We will call these $\{\alpha, \lambda, \delta\}$ respectively. The force will then be periodic with period $\alpha/\lambda + \delta$.

Our integration scheme will thus require us to keep track of the particle's position x. At each step we will calculate $x' = \mathrm{fmod}(x, \alpha/\lambda + \delta)$ (where fmod is the c++ function to compute a remainder of two non-integer numbers) and compute the force (minus the drift) using the following piecewise function:

$$F(x) = \begin{cases} -\lambda & : x' \in [0, \alpha/\lambda] \\ \dfrac{2\alpha}{\delta^2}\left(x - \dfrac{\alpha}{\lambda}\right) & : x' \in [\alpha/\lambda, \delta] \end{cases} \tag{3}$$

The time dependent potential will be a 'ratchet' potential which we will describe with two parameters, τ, τ'. The total period of the ratchet potential is $\tau + \tau'$. To integrate the time dependent dynamics, at each step we will compute $t' = \mathrm{fmod}(t, \tau + \tau')$ and compute the force by:

$$\widetilde{F}(x,t) = \begin{cases} F(x) & : t' \in [0, \tau] \\ 0 & : t' \in [\tau, \tau + \tau'] \end{cases} \tag{4}$$

To truly mimic the Brownian motor, we need to choose parameters such that the particle is virtually unable to cross the barrier height α when the asymmetric potential is turned on. To determine suitable parameters, we can imagine placing a particle in a potential well whose value is given by $U(x)$, but with the quadratic potential extended to infinity on the RHS. The stationary distribution will be given by:

$$\begin{aligned} P^*(x) &\propto \exp\left[\int^x \frac{v(x')}{d}\mathrm{d}x'\right] \propto \exp\left[-\int^x \frac{1}{d}\frac{\mathrm{d}U}{\mathrm{d}x'}\mathrm{d}x'\right] \\ &\propto \exp\left[-\frac{U(x)}{d}\right] \end{aligned} \tag{5}$$

For a particle at the bottom of the well, the rate at which it will transition to a height $\Delta U = \alpha$ up the quadratic barrier is dependent only on the potential difference under Kramer's theory of barrier crossing, and given by:

$$r \propto \exp\left[-\frac{\Delta U}{d}\right] \tag{6}$$

We need $\alpha \gg d$ such that the particle cannot cross the barrier except when the asymmetric potential is turned off [3]. Figures 1 and 2 demonstrate that the particle cannot cross the barrier in the absence of the ratchet potential.

We postulate that the optimal switching time τ will be related to the MFPT for a Brownian particle in a linear potential to travel to the bottom of the slope. This quantity is easily computed by solving the backward Kol-

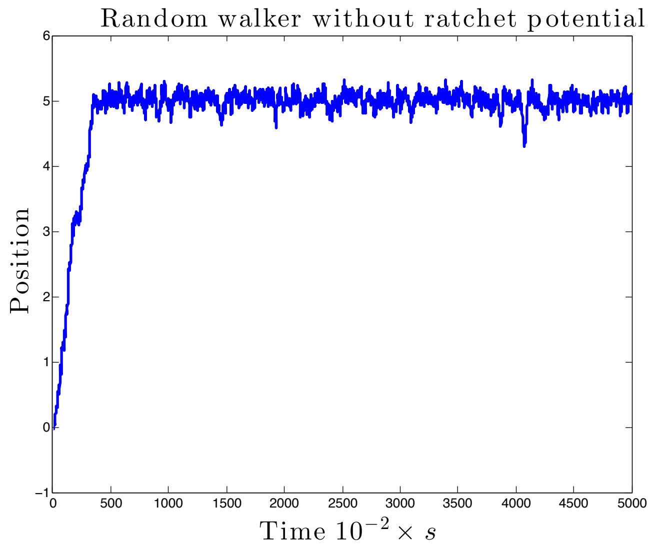

FIG. 1. Without the ratchet potential (i.e. only in the presence of the asymmetric potential) the particle cannot cross the barrier. Here and below, $\alpha = 5, \delta = 1, d = .1, \lambda = 1$.

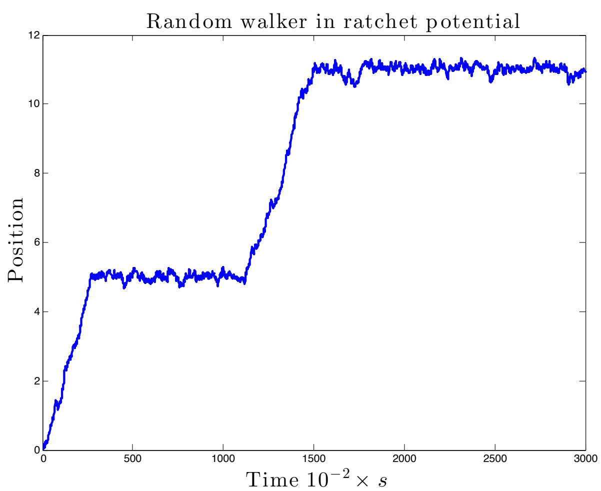

FIG. 2. The ratchet mechanism allows the particle to cross the barrier.

mogorov equation with an absorbing surface at $x = \alpha/\lambda$:

$$-1 = \lambda \frac{\partial}{\partial y}\langle \tau(y) \rangle + d\frac{\partial^2}{\partial y^2}\langle \tau(y) \rangle, \ \langle \tau(\alpha/\lambda) \rangle = 0 \Rightarrow$$
$$\langle \tau(y) \rangle = -\frac{y}{\lambda} + \frac{\alpha}{\lambda^2} \tag{7}$$

and the MFPT at $y = 0$ is α/λ^2. The above result is quite different from that derived by Cox [4] for first passage times in constant drift. Here we have only considered one absorbing state, and simulations show that indeed the above formula is correct. By consider the Euler integration scheme, the mean first passage time simply states

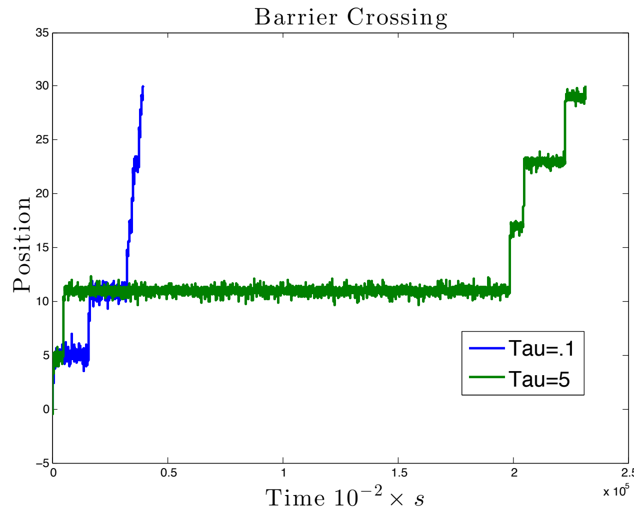

FIG. 3. Here, the expected time for the particle to travel down the sloped portion of the potential is 5s. However, because $\tau' < \tau^*$, clearly a much faster switching rate is optimal. In this picture we consider the time it takes for a particle to travel a distance of 5 steps.

that in expectation the random diffusion terms are zero and the particle travels a distance $\lambda\delta t$ in time δt.

We will numerically determine the optimal switching time τ by plotting the MFPT for the brownian particle to travel N increments along the sawtooth potential (where 'increment' refers to one unit of $\alpha/\lambda+\delta$, the period of the asymmetric potential) as a function of switching time τ.

Note that there is an important parameter that will make an impact in the optimal switching time τ, namely the time scale τ' during which the asymmetric potential is turned off and during which particle can freely diffuse. We note that if τ' is 'too short' such that (in expectation) the random walker is unlikely to cross the restoring portion of the potential barrier, this will lead to an optimal switching time τ which is actually less than the expected MFPT for the random walker to go the length of the step. If $\tau' < \tau^*$ (the time that exactly sets the expected rms displacement to δ in the absence of drift), the particle will likely be stuck at one 'step' for several time periods of the potential ratchet. In this case, the optimal strategy should be to have a very fast τ such that the particle does not spend too much time waiting at the step. Essentially, a very fast τ will give the particle many independent tries to diffuse a distance equal to δ in the short time it has (figure 3).

However, if the diffusion time τ' is sufficiently long that the particle is very likely to cross the distance δ we expect that the rate limiting step will be the time it takes for the particle to travel down the length of the step. In this case, the switching rate should equal the MFPT for the particle to travel down one step. The value of τ^* should be roughly $\delta^2/2D$.

II. OPTIMAL τ GIVEN τ'

We now seek to find the optimal value of τ given a value of τ'. Note that in theory one can simultaneously find an optimal pair τ, τ' by considering exactly the mean first passage times for the particle to diffuse down the step when the asymmetric potential is turned on, and then cross the distance δ when the asymmetric potential is turned off. However, a more interesting problem arises when we consider how τ must compensate for the value of τ'.

For a particle that begins at the top of the linear potential, how long will it take for the particle to reach the bottom of the well as a function of τ, τ' and other model parameters? This problem can be recast as the expected number of periods $\tau + \tau'$ that it will take the particle to reach the bottom. In general, there will be many factors to consider in this calculation, but we can reach an analytical result in certain regimes, for instance if we assume that when the potential is turned off, the particle will diffuse over length scales sufficiently smaller than when the potential is turned on.

We note that the expected displacement when the potential is turned on for a time of δt is $\mathbb{E}[\delta x] = \lambda \delta t$, which can be seen by taking expectation directly of the step δx in the Euler integration scheme. Under the assumption above, the expected number of times it will take the particle to reach the bottom is then the ceiling of $\alpha/\lambda^2\tau$ since it must cover a distance of α/λ.

Once the particle has reached the bottom of the well, it stays here until the potential is turned off, at which point it will diffuse δ to the right with a probability

$$p = \frac{1}{2\sqrt{4\pi D\tau'}} \exp\left(-\frac{\delta^2}{4D\tau'}\right) \tag{8}$$

(where the pre factor of 1/2 denotes the equal likelihood of moving to left or right). If the particle does not make it across the restoring portion of the potential when the force is turned off, it will sit at the bottom of the well and wait another τ time to make another try. The number of times N it must attempt this is then geometric with $P(N = k) = (1-p)^k p$ and satisfies $\mathbb{E}[N] = 1/p$. Thus, the expected time it takes the particle to cross one full step is

$$\left(\left\lceil \frac{\alpha}{\lambda^2\tau} \right\rceil + 2\sqrt{4\pi D\tau'} e^{\delta^2/4D\tau'}\right)(\tau + \tau') \tag{9}$$

We can find the optimal switching rate τ_{opt} by considering the behavior in two regimes. If $\tau_{opt} < \alpha/\lambda^2$, we can see that

$$\tau_{opt} = \sqrt{\frac{p\alpha\tau'}{\lambda^2}} \tag{10}$$

Of course, the above equation is not technically correct since the behavior will have discontinuous jumps for changing values of α due to the ceiling function. This will become approximately correct in the limit that α is large, and then we can 'differentiate' the MFPT directly.

However, when $\tau > \alpha/\lambda^2$, the expected time is linear in τ, and thus the optimal switching time for $\tau > \alpha/\lambda^2$ is exactly α/λ^2. Thus, the optimal switching time depends on the value of $p\tau'$:

$$\tau_{opt} = \min\left(\sqrt{\frac{p\alpha\tau'}{\lambda^2}}, \frac{\alpha}{\lambda^2}\right) \tag{11}$$

We thus expect that for $p\tau' < \alpha/\lambda^2$, τ_{opt} should vary as the square root of α, but for $p\tau' > \alpha/\lambda^2$, τ_{opt} should vary linearly with α. Of course, if τ' gets very large, the above approximations will not all hold. For instance, we now must consider the possibility that if the particle has not reached the bottom of the step like potential, when the asymmetric potential is turned off it might stochastically diffuse backwards a large distance.

We do the simulations for values of $p\tau'$ in both regimes. First, for $\tau' = 5$, $D = .1$, and $\delta = 1$, the value of $p\tau' = .605$. Setting $\lambda = 1$ (and varying α between 1 and 10) puts us in the regime for which τ_{opt} should scale as the square root of α. This indeed appears to be the case (figure 4). However, if we keep all parameters the same but set $\tau' = 140$, the value of $p\tau' = 5.184$. Thus, varying α between 1 and 5 should demonstrate a linear relationship between τ_{opt} and α (figure 5). The fit is not very convincing. We suspect that the square root fit will require a larger value of α. Also, the large value of τ' used for the linear regime violates assumptions above as well since the expected rms displacement when the asymmetric potential is turned off is now $\sqrt{2D\tau'} = 5.29$, which is comparable to the size of the asymmetric step.

III. EFFECTS OF DIMENSIONALITY

We can also study the effects of dimensionality. In this case, the force we consider will be a vector in d dimensions whose ith component is given by:

$$F_i(\mathbf{r}) = \begin{cases} -\lambda x_i/|\mathbf{r}| & : |\mathbf{r}| \in [0, \alpha/\lambda] \\ \dfrac{2\alpha x_i}{|\mathbf{r}|\delta^2}\left(|\mathbf{r}| - \dfrac{\alpha}{\lambda}\right) & : |\mathbf{r}| \in [\alpha/\lambda, \delta] \end{cases} \tag{12}$$

The position of the minimum is slightly shifted, but we see that the main effect is to significantly decrease the mean first passage time as we increase dimensionality (figure 6). This is because our choice of drift has been radially outwards. Thus, because the particle essentially has two or three times as many dimensions with which to reach a given radial displacement, it should intuitively happen faster.

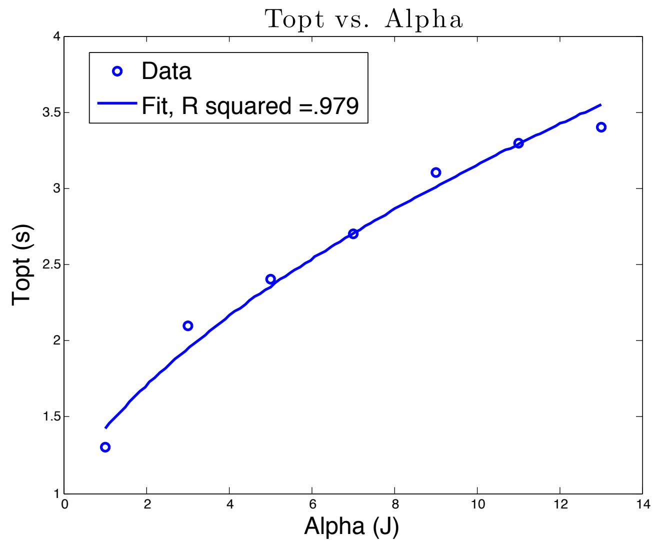

FIG. 4. With this choice of parameters, $p\tau' < \alpha/\lambda^2$ for the full range of α considered, and we see that τ_{opt} varies as the square root of α.

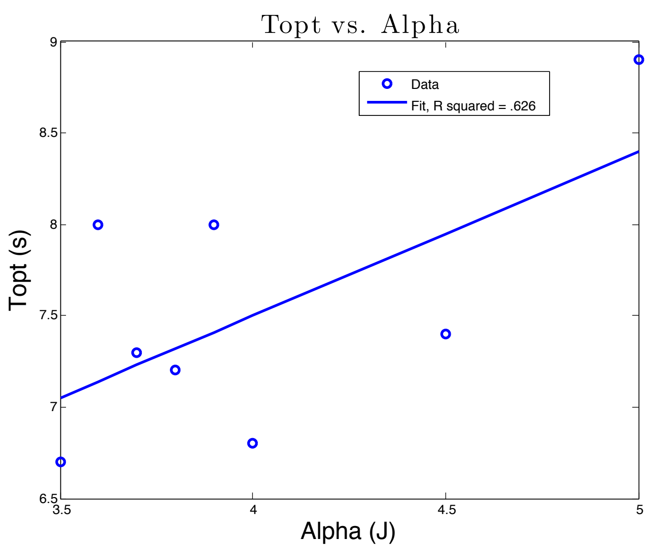

FIG. 5. With this choice of parameters, $p\tau' > \alpha/\lambda^2$ for the full range of α considered. We expect a linear relationship, but presumably τ' is such that some assumptions above have been violated.

RANDOM SWITCHING TIMES

Finally, we may wish to look at how the distribution of waiting times to hit N increments changes when we promote τ, τ' to random variables.

To simulate such a scenario, we will use a mixed stochastic simulation/Euler integrator. We will assume the switching times t, t' to be exponentially distributed random variables with parameter $1/\tau, 1/\tau'$. First, we will choose the time to the next switching event using the inverse CDF of the exponential:

$$t = \tau \ln\left(\frac{1}{U}\right), \qquad t' = \tau' \ln\left(\frac{1}{U}\right), \qquad U \sim \text{Uniform}(0,1) \tag{13}$$

We then time slice the intervals into steps of size $\mathrm{d}t$ and use an Euler integration scheme with the appropriate drift term depending on the ratchet potential.

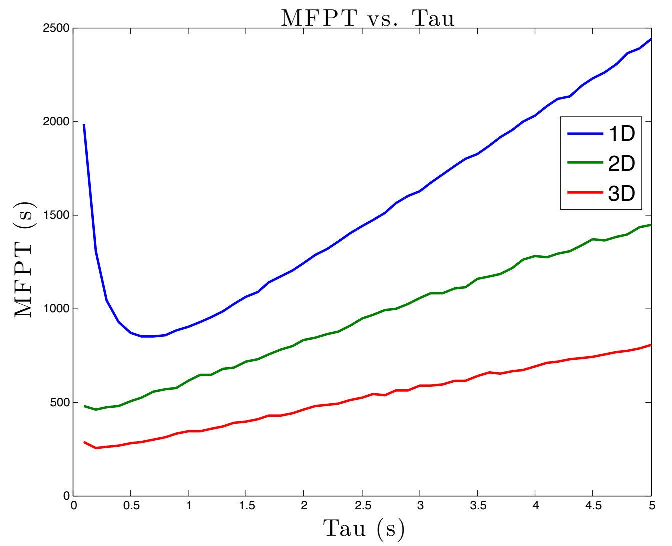

FIG. 6. Here we again consider the MFPT for the particle to travel 5 increments along the potential. The times are greatly reduced as we increase dimensionality, but the location of the minimum shifts only slightly

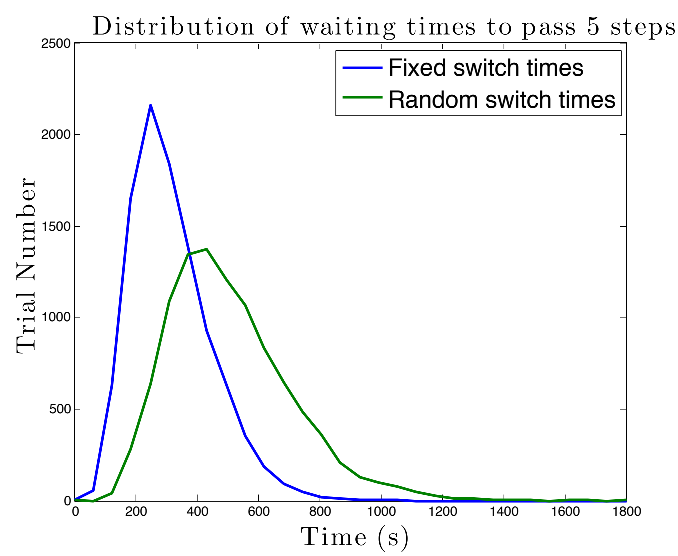

FIG. 7. Histogram of trials to determine the distribution of waiting times for the particle to cross 5 steps. Blue is with fixed switching rates and green curve shows trials in which both τ and τ' are random exponentially distributed variables.

The effect of random switching rates seems only to shift the mean passage time to a larger time, and to add considerable weight to the right tail (figure 7). More work must be done to explain the mechanism for this.

CONCLUSION

We have analyzed the optimal switching time for Brownian motors as a function of model parameters. There is a complex dependence of the optimal switching time τ on the free diffusive time τ' and the distance δ over which the particle must freely diffuse. We have seen that based on changing the value of $p\tau'$ we can significantly change the scaling of τ_{opt} with α. We have analyzed the effects of dimensionality and seen that increasing dimensionality serves mainly to decrease the MFPT to pass N increments along the asymmetric potential. We have seen that promoting the switching times to exponentially distributed random variables will only serve to add weight to the right tail.

[1] M.T. Downton and M.J. Zuckermann, Chaos **15**, 026111 (2006).

[2] Machura et. al, arxiv:cond-mat/0505248v3 (2006)

[3] Moss, (1991). Stochastic Resonance: A signal + Noise in a Two State System. *Forty-Fifth Annual Symposium on Frequency Control.*

[4] Cox, D.R. and Miller, H.D. *The Theory of stochastic processes*. New York: John Wiley & Sons Inc., 1965.