The Langevin equation in 2D for flashing and traveling ratchets

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Abstract: We simulate the Langevin equation in 2D for forces coming from two different type of potentials: flashing and traveling. These potentials produce the so-called ratchet effect, a phenomenon of directed transport in a spatially periodic system. We compare our results with a real experiment in the traveling case and we analyze how the average velocities and diffusions in the canonical directions depend on the potential parameters: a period time τ in the flashing ratchet and a velocity v in the traveling ratchet.

I. INTRODUCTION

The botanist R. Brown observed in 1827 that pollen grains suspended in a fluid execute random and irregular movements. In 1905, Einstein explained this erratic movement as the consequence of the random collisions of the fluid molecules with the Brownian particle. He also developed the first mathematical treatment of the problem. Einstein considered that the motion of the molecules of liquid was so complex that its effects on the pollen grain could only be studied probabilistically in terms of their very frequents (and statistically independent) collisions. Therefore, instead of studying the trajectory of an individual particle, Einstein focused on a probabilistic description valid for an ensemble of Brownian particles: he deduced an equation for the probability density function $P(\vec{x}, t)$ of finding a particle in $\vec{x}$ at time t:

$$\frac{\partial P(\vec{x}, t)}{\partial t} = D\nabla^2 P(\vec{x}, t), \tag{1}$$

which is the same diffusion equation than in physics of continuous matter for the density ρ of soluble substance in a fluid. From the previous equation we can obtain

$$\langle \vec{x}^2(t)\rangle \to 6Dt, \tag{2}$$

which becomes $\langle x^2(t)\rangle \to 2Dt$ in one dimension.

In 1908, Langevin considered a different approach to the problem. He focused on the trajectory of a single Brownian particle and used Newton's second law, adding a sort of fluctuating force $\vec{\xi}(t)$ to describe the highly irregular movement:

$$m\frac{\mathrm{d}\vec{v}}{\mathrm{d}t} = -\gamma\vec{v} + \vec{\xi}, \tag{3}$$

where γ is the friction coefficient (Stokes friction).

Langevin made two assumptions about $\vec{\xi}(t)$: it has zero mean (because collisions occur with the same probability in any direction) and it is uncorrelated to the actual position of the Brownian particle (the molecules of fluid act on the Brownian particles regardless of location), that is:

$$\langle\vec{\xi}(t)\rangle = 0, \qquad \langle\vec{x}\cdot\vec{\xi}\rangle = \langle\vec{x}\rangle\cdot\langle\vec{\xi}\rangle = 0 \tag{4}$$

Langevin also assumed that thermal equilibrium between the Brownian particle and the surrounding fluid has been reached, and then the equipartition theorem implies that $\langle m\vec{v}^2/2\rangle = 3k_BT/2$, where T is the fluid temperature. Multiplying both sides of (3) by $\vec{x}$, taking averages and using the previous considerations, we can get $\langle\vec{x}^2\rangle \to \frac{6k_BT}{\gamma}t$. Comparing with (2), we get then the Einstein relation:

$$D = \frac{k_BT}{\gamma}. \tag{5}$$

If we include a constant force $\vec{F}$, then the mean velocity is

$$\langle\vec{v}\rangle = \frac{\vec{F}}{\gamma}. \tag{6}$$

Remember that a stochastic process is a collection of random variables $\{x(t), t \geq 0\}$ indexed by time. The most famous one is the Wiener process, W, which can be caracterized by giving its mean value and the two-times correlation function:

$$\langle W(t)\rangle = 0, \quad \langle W(t_1)W(t_2)\rangle = \sigma^2 \min(t_1, t_2). \tag{7}$$

The derivative of the Wiener process (in a sense explained in [1]) is precisely $\xi(t)$, which is a Gaussian process with

$$\langle\xi(t)\rangle = 0, \quad \langle\xi(t_1)\xi(t_2)\rangle = 2\delta(t_1 - t_2). \tag{8}$$

known as white noise. In 2D, it is $\vec{\xi}(t) = (\xi_x(t), \xi_y(t))$, where ξ_x and ξ_y are independent white noises.

The purpose of this document is to study the Langevin equation in 2D when there is a force $\vec{F} = -\vec{\nabla}V$ derived from a time-dependent potential in the so-called overdamped regime. If collisions occur at a characteristic time τ_{coll}, the Langevin equation description applies at times $t \gg \tau_{coll}$. It takes the form:

$$m\ddot{\vec{r}} = -\vec{\nabla}V - \gamma\dot{\vec{r}} + \vec{\eta}, \tag{9}$$

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where $\vec{\eta}(t) = \sqrt{\gamma k_B T}\vec{\xi}(t)$ is the random force which gives the fluctuations. The constant $\gamma k_B T$ is determined by using the fact that, at times $t \gg 1/\gamma$, the system gets relaxed to equilibrium and the equipartition theorem holds.

For micron-sized colloid, the Reynolds number is very small and the inertial effects (captured by $m\dot{v}$) can be disregarded. That is what we call the overdamped regime. From the equation (9), we get

$$\dot{\vec{r}}(t) = -\frac{1}{\gamma}\vec{\nabla}V(\vec{r}(t),t) + \sqrt{\frac{k_B T}{\gamma}}\,\vec{\xi}(t). \tag{10}$$

This equation of motion can be integrated numerically, up to order h (the integration time step), with the stochastic Milshtein algorithm [1]:

$$\vec{r}(t_{i+1}) = \vec{r}(t_i) - \frac{1}{\gamma}h\vec{\nabla}V(\vec{r}(t_i),t_i) + \sqrt{2\frac{k_B T}{\gamma}h}\,\vec{u}_i, \tag{11}$$

where, for every i, $\vec{u}_i = (u_i^x, u_i^y)$ is a vector of two independent Gaussian random variables with mean 0 and variance 1 and the vectors in the set $\{\vec{u}_i\}$ are independent.

We will study this equation numerically in 2D for forces F coming from ratchet potentials. The ratchet effect is a phenomenon of directed transport in a spatially periodic system. As explained in [2], in general, the directed transport may be achieved by breaking the spatial inversion symmetry and the time symmetry. It is possible with periodic and asymmetric potentials, the so-called ratchet potentials.

We will work with two kinds of ratchet potentials. Firstly, we will study how the particles behave under a flashing potential. Secondly, we will use a traveling potential taking [3] as a reference, where the authors modulate by an oscillating magnetic field the parallel magnetic stripes of a ferrite garnet film (FGF), resulting in a directed transport perpendicularly to the stripes. In their experiments, they use polystyrene paramagnetic particles diluted in deionized water and moving on top on the FGF. In that case, according to [4], the particles motion is basically confined to the $x-y$ plane and there is a net force along the x-axis coming from a traveling potential $V(x,t)$. In the y-axis, the forces are negligible. Although that our simulation will be simpler, we expect similar results. In particular, we should obtain a net velocity in the x-axis and no relevant velocity in the y direction. We will compare the trajectory of a single particle in our simulation with the real results of the experiments in [3]. In both cases, we will study how the average velocities $\langle v_x\rangle$, $\langle v_y\rangle$ and diffusions $\langle D_{xx}\rangle$, $\langle D_{yy}\rangle$ of the particles depend on a parameter of the potential (the time period in the flashing ratchet and the traveling velocity in the traveling ratchet).

II. FLASHING AND TRAVELING RATCHETS

Firstly, we study a simple case of a flashing potential. We consider a periodic and ratchet potential V that is periodically flashing on and off. When V is applied, particles are trapped in the minima of the potential. We suppose that our particles are initially near to the central minimum, as shown in Fig. 1. Then we have a distribution centered at the minimum due to the random fluctuations. When the potential is off, the particles diffuse freely and the variance of the concentration increases because of the diffusion. Once the potential is switched on again, the particles that are located at the right of αL move forwards to the minimum at L. It happens with a probability P_{right} that is proportional to the orange area. Equally, there is a probability P_{left}, proportional to the blue area, that some particles are to the left of $-(1-\alpha)L$ and then move backward to the minimum at $-L$. Since the orange area is larger than the blue area, $P_{\text{right}} > P_{\text{left}}$ and it is more likely to be trapped in the well at L than at $-L$. Therefore, the asymmetry of the potential creates a net displacement of the particles to the right. Obviously, the symmetric case ($\alpha = 1/2$) does not yield a preferential direction.

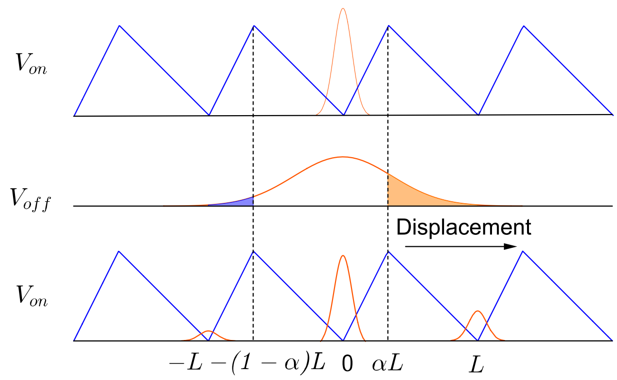

FIG. 1: A flashing potential, with $\alpha = 1/3$.

Next we consider a traveling potential ratchet in x-axis:

$$V_1(x,t) = V_1(x - vt, t) \tag{12}$$

where v is the traveling velocity. In this case, as the minima of the potential are moving in the traveling velocity direction, the particles are dragged in the same direction. We suppose that our particles are initially trapped near to a single minimum (see Fig. 2). As time goes on, the minimum is moving forward and then our distribution around this minimum is forced to move to the right. Nevertheless, we will see that the real behaviour is not always so simple.

We will add to both potentials a periodic 2D fixed potential, which consists in periodic minima and maxima in a square configuration:

$$V_2(x,y) = V_2^0\left(1 + \sin\left(\frac{2\pi x}{\lambda}\right)\sin\left(\frac{2\pi y}{\lambda}\right)\right). \tag{13}$$

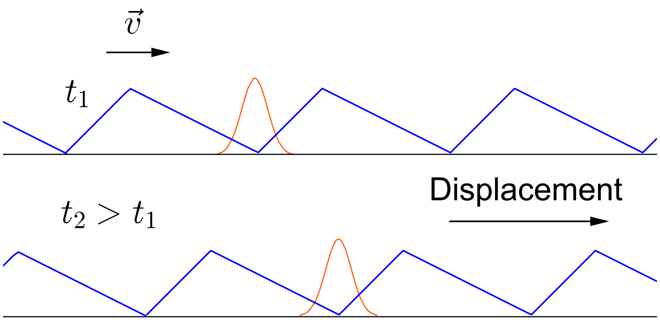

FIG. 2: A traveling potential, moving to the right.

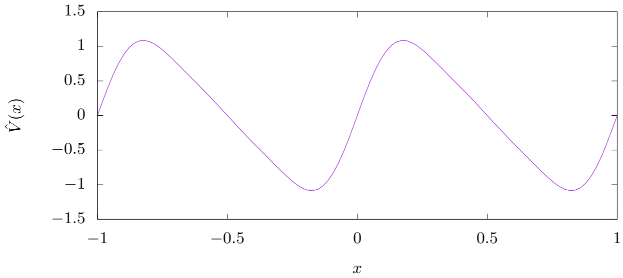

FIG. 3: $\hat{V}(x)$.

III. RESULTS

We have simulated the Langevin equation in 2D for forces coming from two potentials:

$$V\left(x',y',t'\right) = V'_{10}\,\hat{V}_1\left(x',t'\right) + V'_{20}\,\hat{V}_2\left(\frac{x'}{\lambda'},\frac{y'}{\lambda'}\right) \quad (14)$$

where the first term will be a flashing or traveling potential. To simplify the simulation, we have used a standard nondimensionalization method for the equation (10) with the previous potential. For example, if

$$V_1\left(x',t'\right) = V_1\left(\frac{x'}{\lambda'},\omega' t'\right), \quad (15)$$

as will be the case in our flashing potential, we can define the following dimensionless variables:

$$x = \frac{x'}{\lambda'}, \qquad y = \frac{y'}{\lambda}, \qquad t = \frac{t'}{t_0}, \quad (16)$$

where t_0 is an auxiliar constant such that $t_0 V'_{10}/\gamma\lambda'^2 = 1$. If we define the following dimensionless parameters,

$$\omega = \frac{\gamma\lambda'^2}{V'_{10}}\omega', \qquad \hat{T} = \frac{k_B}{V'_{10}}T, \quad (17)$$

the two-dimensional equation (10) becomes

$$\begin{aligned} \dot{x} &= -\frac{\partial \hat{V}_1}{\partial x}(x,\omega t) - \frac{V'_{20}}{V'_{10}}\frac{\partial \hat{V}_2}{\partial x}(x,y) + \sqrt{\hat{T}}\,\xi_x \\ \dot{y} &= -\frac{\partial \hat{V}_2}{\partial y}(x,y) + \sqrt{\hat{T}}\,\xi_y, \end{aligned} \quad (18)$$

where all variables and parameters are dimensionless.

The traveling potential can be treated in a very similar way. In this case, the potencial has the form

$$V_1\left(x',t'\right) = V'_{10}\,\hat{V}_1\left(\frac{x'-v't'}{\lambda'}\right), \quad (19)$$

where v' is the traveling velocity. Following an analogous process and defining $v = \frac{\gamma\lambda'}{V'_{10}}v'$, one can arrive to the corresponding dimensionless Langevin equations, like in (18).

As we have just seen, we can take our potentials as $V(x,y,t) = V_1(x,t) + V_2(x,y)$, where x, y, t are dimensionless variables. The potential V_2 has already been stated at (13). In the next section, we will specify the potentials that we have used.

We have supposed an initial condition $(x_0, y_0) = (0,0)$ and we have taken $\hat{T} = 0.2$. The simulations have been applied to ensembles of $N = 400$ particles; the results shown below are always the average quantities of these collections at large enough times ($t = 1000$). In fact, the definitions of velocity and diffusion are

$$\begin{aligned} \langle v_x\rangle &= \lim_{t\to\infty}\frac{\langle x(t)\rangle}{t}, \quad \langle D_{xx}\rangle = \lim_{t\to\infty}\frac{\langle x^2(t)\rangle - \langle x(t)\rangle^2}{t}; \\ \langle v_y\rangle &= \lim_{t\to\infty}\frac{\langle y(t)\rangle}{2t}, \quad \langle D_{yy}\rangle = \lim_{t\to\infty}\frac{\langle y^2(t)\rangle - \langle y(t)\rangle^2}{2t}. \end{aligned}$$

It is important to ensure that the time we take is much longer than any other characteristic time of the system, as explained in [5].

A. Flashing potential

We set $V_2^0 = 0.1$ and $\lambda = 0.5$ in (13) and let $V_1(x,t)$ be the following flashing potential:

$$V_1(x,t) = f(t)\hat{V}(x), \quad (20)$$

with $\hat{V}(x) = [\sin(2\pi x) + 0.25\sin(4\pi x) + 0.05\sin(6\pi x)]$ and $f(t) = (1+\cos(\omega t))/2$, where $\omega = 2\pi/\tau$ and τ is the time period. We graph $\hat{V}(x)$ in Fig. 3.

According to the previous section, there should be a finite and positive average velocity in the x-axis, $\langle v_x\rangle > 0$. That is, the particles are transported forward by the flashing potential. In contrast, we do not expect a net velocity in the y-axis, because the potential $V_2(x,y)$ does not give any preferential direction. These physical intuitions are verified in Fig. (4), where we represent the statistical averages velocities in directions x and y depending on the parameter τ. We clearly observe a peak around $\tau = 0.4$ in $\langle v_x \rangle$ from which velocity starts to decrease to 0. For very small τ, that is, in the case that the potential is flashing very quickly, a particle trapped in a minimum of the potential does not have time to diffuse enough when the potential is off (or has a small amplitude) to escape this potential well. Since the particles are confined, $\langle D_{xx} \rangle$ is close to 0. For the same reason, as τ increases, we expect that $\langle v_x \rangle > 0$ and $\langle D_{xx} \rangle$ increases. However, for large τ, the potential amplitude changes slowly and then the directed transport takes place at low velocity. Therefore, there must be a optimal time period τ. We also observe that $\langle D_{yy} \rangle \approx 0.2$, which is the value of $\hat{T}$. It is coherent with [5]. We also see that $\langle D_{xx} \rangle < \langle D_{yy} \rangle$; it may happen because, while the particles are dragged forward in the x-axis by the flashing potential, they diffuse freely in the y-axis, so it seems reasonable a larger diffusion in the y direction.

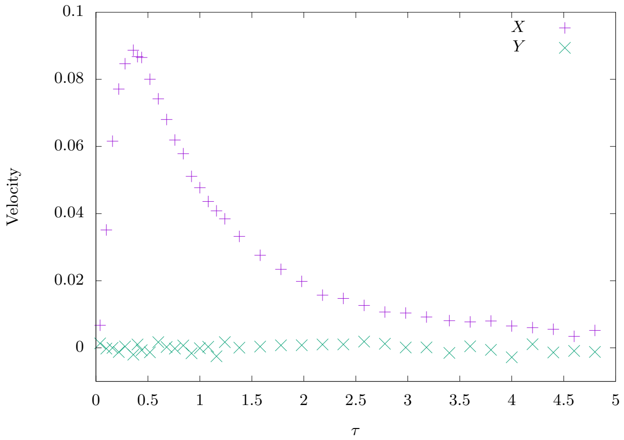

FIG. 4: Average velocities in x-axis and y-axis, $\langle v_x \rangle$, $\langle v_y \rangle$, versus the period time τ, after a time $t = 1000$.

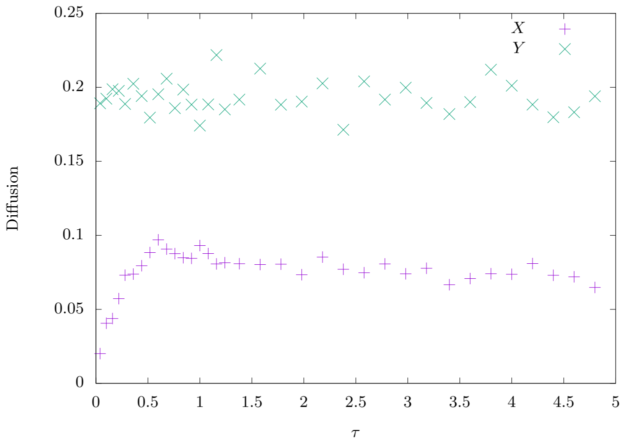

FIG. 5: Average diffusions in x-axis and y-axis, $\langle D_{xx} \rangle$, $\langle D_{yy} \rangle$, versus the period time τ, after a time $t = 1000$.

B. Traveling potential

Now we take the potential $\hat{V}(x)$, but we replace x by $\bar{x} = x - vt$, where the velocity v is a parameter. Then we get a traveling potential:

$$V_1(x,t) = \sin(2\pi\bar{x}) + 0.25\sin(4\pi\bar{x}) + 0.05\sin(6\pi\bar{x}), \quad (21)$$

where $\bar{x} = x - vt$. We set $V_2^0 = 0.5$ and $\lambda = 1$ in (13).

Now we compare the trajectory of a single particle under the potential $V(x, y, t)$ with the following figure extracted from [3]:

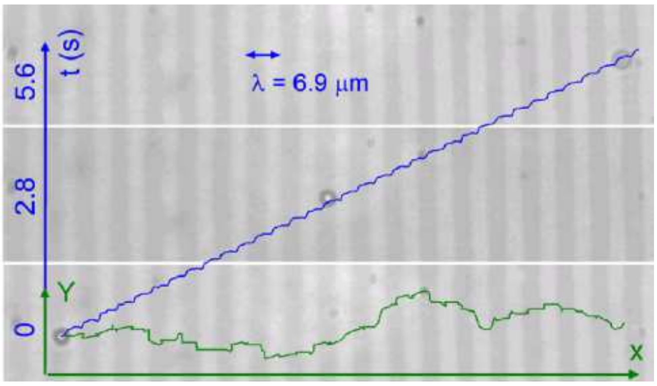

FIG. 6: Particle trajectory $x(t)$ and its corresponding path in the $x - y$ plane, extracted from [3].

Our equivalent graphic is Fig. 7, with slightly different axis. As expected, our simulation gives similar results to Fig. 6. We have a net velocity in the x-axis and fluctuations around 0 in the y direction.

We graph in Figs. 8, 9 velocities and diffusions in x and y depending on the traveling velocity v. As expected, there is a net velocity in x. Nevertheless, like in flashing ratchet, there is a peak in this case around $v = 3.4$ in $\langle v_x \rangle$. This fact agrees with the experiments in [6], where the author detect that above a critical velocity the overdamped

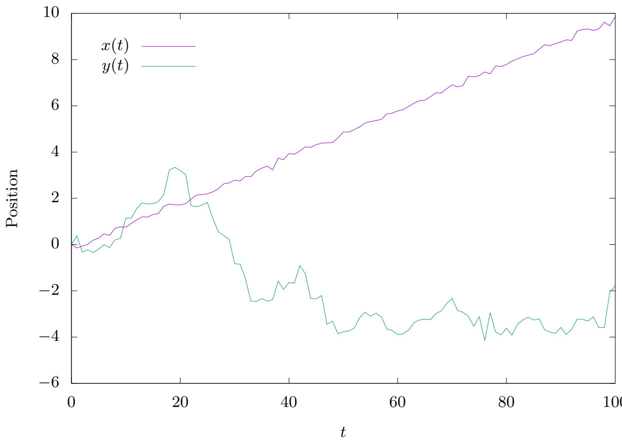

FIG. 7: A single particle trajectory $x(t)$ and $y(t)$, for a velocity parameter $v = 0.1$.

particles are unable to follow ratchet modulations. Diffusion in y-axis, $\langle D_{yy} \rangle$ fluctuates around $\hat{T} = 0.2$, as expected, and we observe that there is a maximum for $\langle D_{xx} \rangle$ near to the critical velocity.

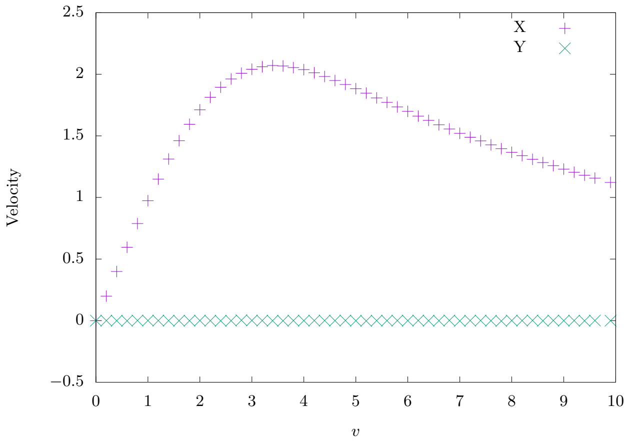

FIG. 8: Average velocities in x-axis and y-axis, $\langle v_x \rangle$, $\langle v_y \rangle$, versus the velocity v, after a time $t = 1000$.

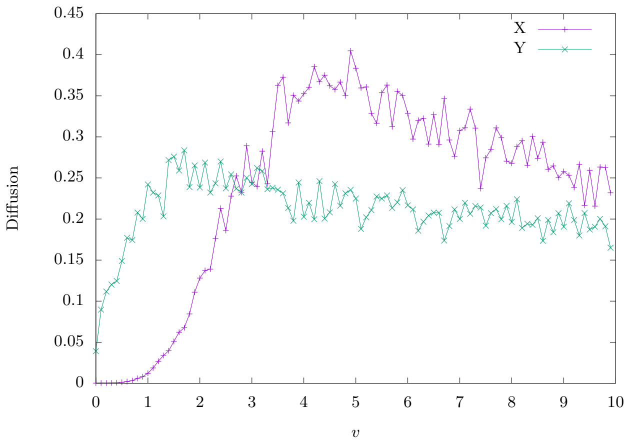

FIG. 9: Average diffusions in x-axis and y-axis, $\langle D_{xx} \rangle$, $\langle D_{yy} \rangle$, versus the velocity v, after a time $t = 1000$.

IV. CONCLUSIONS

In this essay, we have shown that a Brownian particle under a so-called ratchet potential experiences the ratchet effect, a directed transport due to the break of spatial and time symmetry. We have seen it by simulating the Langevin equation -previously nondimensionalized- in 2D with the stochastic Milshtein algorithm.

In the flashing potential case, we have shown that $\langle v_x \rangle$ has a peak around $\tau = 0.4$. In contrast, $\langle v_y \rangle \approx 0$, because the potential does not give any preferential direction in the y-axis. In the traveling potential case, the results for a single particle trajectory are consistent with [3], the article which has inspired this part of our work. As expected, we have observed a net velocity in the traveling direction, x-axis, and fluctuations in the y-axis, where the potential does not give any preferential direction. Furthermore, we have seen a peak around $v = 3.4$, a critical velocity from which the overdamped particle can not follow the potential. This peak appears in a similar form in the article [6]. The diffusion $\langle D_{xx} \rangle$ has a maximum near to the critical velocity and $\langle D_{yy} \rangle$ has a value close to $\hat{T}$ in both potentials, as predicted in [5].

To take further this work, we should be more careful about the parameters. We should fix them according to the real conditions of the problem that we pretended to study. Despite this, this work has been useful as a first approach to the Langevin equations and the ratchet potentials.

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