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Ratchet, pawl and spring Brownian motor

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Abstract

We present a model for a thermal Brownian motor based on Feynman's famous ratchet and pawl device. Its main feature is that the ratchet and the pawl are in different thermal baths and connected by a harmonic spring. We simulate its dynamics, explore its main features and also derive an approximate analytical solution for the mean velocity as a function of the external torque applied and the temperatures of the baths. Such theoretical predictions and results from numerical simulations agree within the ranges of the approximations performed.

Keywords: Brownian motor; Feynman's ratchet; Nonlinear Langevin equations

1. Introduction

Engines that aim to do useful work by rectifying thermal fluctuations are called Brownian motors (BM). During the last few years a lot of effort has been invested in studying the underlying mechanism of such engines, which has been called the ratchet effect [1]. This is a mechanism that consists of breaking the spatial and temporal inversion symmetry of the system so that directed transport emerges, thermal fluctuations being very relevant input. In fact, the paradigmatic device of such speculation is Feynman's famous ratchet and pawl machine [2].

In 1963 Feynman introduced [2] a microscopic device (the ratchet and pawl machine) that can operate between two thermal baths extracting some mechanical work. The hotter bath contains an axle with vanes in it. The bombardment of gas molecules on the vane make the axle rotate with random symmetric fluctuations. At the other end side of the axle, as shown in Fig. 1, there is a second box with an asymmetric toothed wheel which, in principle, can turn only one way due to a coupling with the pawl (the stopping mechanism).

At first glance, one could think that it seems quite likely that the wheel will spin round one way and lift a weight even when both gases are at the same temperature, thus violating the Second Law. However, a closer look at the pawl reveals that it bounces, so the wheel will rotate randomly in any direction, doing a lot of jiggling but with no net turning. Thus, the machine cannot extract work from two baths at the same temperature. When the temperature of the vanes is higher than the temperature of the wheel, Feynman concludes that some work is performed with Carnot's efficiency when the machine is lifting the weight very slowly. This is indeed a very optimistic result, which has been revised, many years later, in Refs. [3, 4]. Such particular device has been analyzed and it has been suggested that this engine is very far from Carnot efficiency [3] due to the fact that this type of device has strong heat losses. A more refined analysis and modeling of Feynman's motor has been presented in several references [4–7], with the conclusion that its efficiency is very poor. The main problem comes from the mechanical coupling of the pawl mechanism, which is not very efficient. The microscopic analysis of a thermal Brownian motor in Ref. [8] is very illuminating for clarifying the principles underlying the Feynman ratchet.

Moreover, the main idea underlined in the the ratchet and pawl mechanism can be implemented in different ways. In this work we propose a model through an equation for a dynamical classical variable (position or angle) moving in a periodic and asymmetric potential (a ratchet potential) in a bath at temperature T_1 coupled with another degree of freedom immersed in a different bath at temperature T_2. The coupling mechanism is a harmonic spring. In this case, the two thermal baths are clearly separated and the performance of this engine

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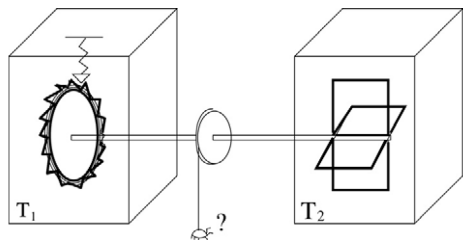

Fig. 1. Feynman's original ratchet and pawl machine.

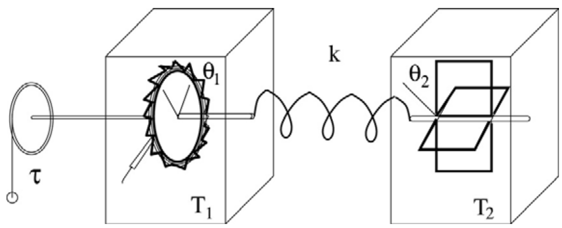

Fig. 2. Ratchet, pawl and spring Brownian motor.

can be studied as a function of the different parameters. In the following section, we introduce the model. Once the model is explained and justified, in Section 3 we present results by numerical simulation of the stochastic equations of motion. In Section 4, an analytical approach is presented, and in Section 5 we show the agreement of the theoretical expressions found with the data from numerical simulations. Finally, we end with some conclusions and comments.

2. The ratchet, pawl and spring motor Brownian motor (RPSBM)

First of all, let's describe our proposal for a Brownian motor as it is shown in Fig. 2. It consists of two boxes at different constant temperatures. The left box contains a ratchet and a pawl that act like a mechanical rectifier device. From this box, an axle-wheel device is connected, allowing it to lift a hanging object in order to study how much work the device can perform. The second box is at a higher temperature than the first one and has a little windmill that is used to pick up energy from the thermal bath (through collisions of the particles of the bath with the vanes) and to transfer it to the ratchet and pawl system through the spring. The main simplification of our model is that the dented wheel and the pawl mechanisms are substituted by a ratchet potential and a harmonic spring. Then it is straightforward to write the Langevin equations in the over-damped limit:

$$\lambda_1 \frac{d\theta_1}{dt} = -\frac{\partial V_R(\theta_1)}{\partial \theta_1} - k(\theta_1 - \theta_2) - \tau + \xi_1(t), \quad (1)$$

$$\lambda_2 \frac{d\theta_2}{dt} = k(\theta_1 - \theta_2) + \xi_2(t), \quad (2)$$

with thermal noise satisfying the fluctuation–dissipation relation,

$$\langle \xi_i(t)\xi_j(t')\rangle = 2k_B T_i \lambda_i \delta_{ij}\delta(t - t'). \quad (3)$$

Note that we are describing the evolution in time of the angular positions θ_1 and θ_2 of the ratchet and the windmill, respectively.

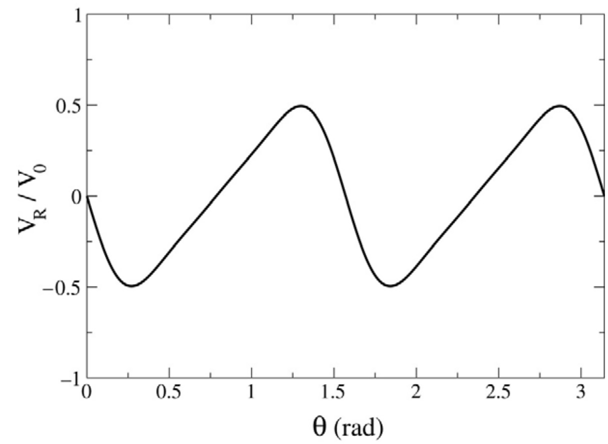

Fig. 3. Shape of the ratchet potential V_R for $d = 4$.

We see in Eq. (1) a force term that comes from a periodic and asymmetric potential V_R that models the shape of the sawtooth wheel. There is also an external torque τ that can be different to zero to account for the work done. Two independent white noises ξ_1 and ξ_2 represent thermal fluctuations and, finally, there is an interaction between the two baths through a harmonic spring of constant k. A linear coupling between both degrees of freedom also appears in Ref. [9].

The ratchet potential $V_R(\theta)$ is given by,

$$V_R(\theta) = -\frac{V_0}{2.23}[\sin(d\theta) + 0.275\sin(2d\theta) + 0.0533\sin(3d\theta)], \quad (4)$$

where V_0 controls the height of the potential, d is the number of teeth per turn, and the asymmetry of the potential is controlled by changing the numerical coefficients that multiply the sine functions. In Fig. 3 we see the explicit form of the ratchet potential $V_R(\theta)$ used in our study.

This problem has a set of parameters that can be simplified if a new time dimensionless scale is defined, $t = \frac{\lambda_1}{V_0}s$. Then Eqs. (1) and (2) are transformed and all the relevant parameters, $\widetilde{T}_1 = \frac{k_B T_1}{V_0}$, $\widetilde{T}_2 = \frac{k_B T_2}{V_0}$, $\widetilde{k} = \frac{k}{V_0}$, $\widetilde{\lambda} = \frac{\lambda_1}{\lambda_2}$ and $\widetilde{\tau} = \frac{\tau}{V_0}$, are now dimensionless. In this way we can concentrate on the main parameters that control the dynamics of the system. For instance, we see that V_0 controls the energy scale, with respect to the thermal energy of the baths.

3. Numerical results and optimal regime of the motor

In this section we present the results by numerically simulating Eqs. (1) and (2). We have used a second order algorithm (Heun), which is a generalization of the Runge–Kutta algorithm for stochastic systems. Since the process is intrinsically nondeterministic, it is convenient to perform statistics in order to minimize fluctuations in the output data. For that reason, we have averaged every step of the integration over 500 different particles. In Fig. 4 we show an example of a single trajectory in time and the mean $\langle\theta_1(s)\rangle$.

We must first explore the role played by every parameter of the model in order to get in scale and tune them cleverly to obtain the most efficient working regime. The height of the

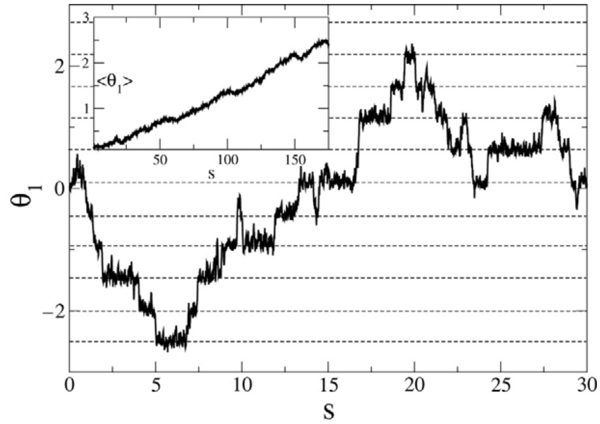

Fig. 4. Typical evolution of the angle position θ_1 as a function of the dimensionless time s obtained directly from the simulations. The parameters are $V_0 = 3k_BT_1$, $k = 100k_BT_1$, $d = 12$ and $T_2 = 2T_1$. Plot of a single trajectory (for $\tau = 0$) in which one can see the discrete jumps of the dynamics from one valley to another of the saw-tooth potential. Inset: average of $\theta_1(s)$ over many particles for $\tau = 0.01k_BT_1$.

potential V_0 is a very relevant parameter, since it determines the energy scale of the system. We are interested in an energy barrier higher than the energies of the two thermal baths but not much more. Otherwise, the engine would not work, because thermal fluctuations would not be able to cause a jump over such a high barrier. There is an optimal value, which is found to be around $V_0 = 3k_BT_1$. For smaller values, the height is too small and thus fluctuations can jump over it to both sides, giving a zero velocity on average. For large V_0, the system is hardly ever able to perform a jump to the next valley. This is what is expected from intuition, and also what is found from numerical simulations.

Regarding temperatures, we must choose T_2 higher than T_1, but not too much because large randomness [10] blurs and destroys directional motion. In a following section, we will analyze in detail the behavior of the mean speed as a function of the ratio of temperatures. In fact, there is an optimal ratio, which is around $T_2 \simeq 4T_1$.

We have also checked that the velocity falls to zero for two limits of the coupling constant: $k \to 0$ and $k \to \infty$. This is in perfect accordance with the following thermodynamical arguments. For k going to zero, the systems are un-coupled and therefore we have a single bath at a constant temperature. In this situation, the wheel will have no mean velocity. For the opposite limit, that is, large values of the coupling constant, we use the argument discussed in Ref. [3]. A very high k is equivalent to having both systems joined by a rigid axle vane. Then, the system is in contact with two thermal baths at different temperatures. One can prove that the system senses a single averaged temperature, and thus it will not run at all on average either.

There seems to be an optimal number of teeth d as well. For low values of d, the wheel is not a proper sawtooth and the asymmetry of the potential is not felt. For d around $d = 24$ we find that the wheel spins more quickly, while for greater d the velocity decays again. Notice that the force term is proportional to the number of teeth. This means than the higher d is, the steeper the potential becomes.

Using three other different models of the ratchet potential, which are built similarly but by modifying the coefficients multiplying the sine functions, we see that the more asymmetrical the model is, the faster the system runs. Obviously, for a symmetric potential, no rectification of the fluctuations is possible for any value of the rest of the parameters.

When examining Eqs. (1) and (2) in dimensionless variables, one finds that the noises, in dimensionless variables too, should be written as

$$\langle \widetilde{\xi}_1(s)\widetilde{\xi}_1(s')\rangle = 2\widetilde{T}_1\delta(s-s'), \tag{5}$$

$$\langle \widetilde{\xi}_2(s)\widetilde{\xi}_2(s')\rangle = 2\widetilde{\lambda}\widetilde{T}_2\delta(s-s'), \tag{6}$$

$$\langle \widetilde{\xi}_1(s)\widetilde{\xi}_2(s')\rangle = 0. \tag{7}$$

Notice that the effective intensity of the second bath is the thermal energy of the bath in terms of V_0 multiplied by the fraction of the friction coefficients.

Finally, when setting $\lambda_1 = \lambda_2$, $T_2 = 2T_1$, $V_0 = 3k_BT_1$, $\tau = 0$, $k = 80k_BT_1$ and $d = 24$, we are in an optimal regime in which the angular velocity is nearly the greatest possible: $v \doteq \langle\dot{\theta}_1\rangle \simeq 0.021\ \mathrm{s}^{-1}$.

Apart from the quantitative numerical value itself, we can draw two main conclusions. The first one is that the engine does work. We have performed some simulations in which we use a torque τ different to zero. For instance, for a small torque $\tau = 0.1k_BT_1$ we see that the systems still runs and lifts the external weight, thus performing useful work. The second conclusion is that this motor is very inefficient. Energetics are not worth calculating in detail because, just by comparison with the model in [5], we can see that the maximum velocity achieved by the RPSBM is at least five times smaller than the speeds found in Ref. [5] for the SBM. Therefore, the efficiency of the present model is much smaller still.

4. Analytical study of the RPSBM

Our purpose now is to undertake an analytical study of our motor. Any kind of exact calculation in such systems seems impossible and, therefore, some approximations have to be assumed.

Consider the equations that define our Brownian motor written in the form

$$\dot{\theta}_1 = f(\theta_1) - k(\theta_1-\theta_2) - \tau + \xi_1(t), \tag{8}$$

$$\dot{\theta}_2 = k(\theta_1-\theta_2) + \xi_2(t), \tag{9}$$

where $f(\theta_1)$ is the force exerted by the ratchet potential: $f(\theta_1) = -V_R'(\theta_1)$. Note that we have set the friction coefficients to one for simplicity, without losing any generality in the calculus. Let us now define the changes of variables

$$x = \frac{\theta_1+\theta_2}{2}, \quad y = \frac{\theta_1-\theta_2}{2}. \tag{10}$$

The relevant variable x describes the evolution of the center of mass and the "irrelevant" variable y describes the relative motion of the two-particle system. The equations of motion in these new variables are

$$\dot{x} = \frac{f(x+y)}{2} - \frac{\tau}{2} + \eta_1(t), \tag{11}$$

$$\dot{y} = \frac{f(x+y)}{2} - \frac{\tau}{2} - 2ky + \eta_2(t), \tag{12}$$

where a redefinition of the noises has been introduced as

$$\eta_1(t) = \frac{\xi_1(t) + \xi_2(t)}{2}, \quad \eta_2(t) = \frac{\xi_1(t) - \xi_2(t)}{2}. \tag{13}$$

Let us make our first approximation. Using the fact that y is very small, we can make a Taylor expansion of $f(x+y)$ up to first order in y, obtaining the pair of equations

$$\dot{x} = \frac{f(x) + yf'(x) - \tau}{2} + \eta_1(t), \tag{14}$$

$$\dot{y} = \frac{f(x) - \tau + y(f'(x) - 4k)}{2} + \eta_2(t). \tag{15}$$

Since numerical simulations indicate that the variable y has faster dynamics, we will eliminate it adiabatically. This means that we set $\dot{y} \doteq 0$. Then Eq. (15) reduces to

$$y = \frac{1}{4k - f'(x)}[f(x) - \tau + 2\eta_2(t)]. \tag{16}$$

One can see that the term $4k$ is much bigger than $f'(x)$ when $k \simeq 100k_B T_1$ and d is small ($d \simeq 4$). Then, within this range of parameters, we can keep only $4k$ in the denominator. Now substituting the last expression for y in Eq. (14), we end up with a Langevin equation with a new force $H(x)$ and two multiplicative noises $g_1(x)$ and $g_2(x)$,

$$\dot{x} = H(x) + g_1(x)\xi_1(t) + g_2(x)\xi_2(t), \tag{17}$$

where,

$$H(x) = \frac{1}{2}(f(x) - \tau)\left(1 + \frac{f'(x)}{4k}\right), \tag{18}$$

$$g_1(x) = \frac{1}{2}\left(1 + \frac{f'(x)}{4k}\right), \quad g_2(x) = \frac{1}{2}\left(1 - \frac{f'(x)}{4k}\right). \tag{19}$$

The Fokker–Planck equation associated with Eq. (17) is

$$\partial_t P(x,t) = -\partial_x J(x,t), \tag{20}$$

where

$$J(x,t) = H(x)P(x,t) - k_B T_1[g_1(x)\partial_x g_1(x)P(x,t)] - k_B T_2[g_2(x)\partial_x g_2(x)P(x,t)]. \tag{21}$$

After some manipulations with partial derivatives, the probability current $J(x,t)$ can be rewritten as

$$J(x,t) = H(x)P(x,t) - [g_{\mathrm{eff}}(x)\partial_x g_{\mathrm{eff}}(x)P(x,t)], \tag{22}$$

with

$$g_{\mathrm{eff}}(x) = \sqrt{k_B T_1 g_1^2(x) + k_B T_2 g_2^2(x)}. \tag{23}$$

Since we are interested in the steady state, we now have to solve Eq. (22) for a constant probability current J. The first step is to reduce this equation to a Bernoulli form that can formally be integrated. By imposing periodic boundary conditions, $P(x) = P(x+L)$, where $L = \frac{2\pi}{d}$, we find that

$$P_0(1 - \mathrm{e}^{\beta(L)}) = J\int_0^L \mathrm{d}x \frac{\mathrm{e}^{-\beta(x)}}{g_{\mathrm{eff}}(x)}, \tag{24}$$

where P_0 is a constant that can be found from the normalization condition $\int_0^L P(x)\,\mathrm{d}x = 1$, and β is a relevant function whose expression is

$$\beta(x) = \int_0^x \mathrm{d}x' \frac{-H(x')}{g_{\mathrm{eff}}^2(x')}. \tag{25}$$

The mean velocity $v \doteq \langle\dot{x}\rangle$ is just the integral of the probability current over the spatial period L. Since J is constant, we have from Eq. (24) that the solution for v is [11–15]

$$v = \mathcal{N}(1 - \mathrm{e}^{\beta}), \tag{26}$$

where $\mathcal{N}$ is a constant that is found by using the normalization condition for the probability $P(x)$. We will see that this constant depends very smoothly on the control parameters of our model. Notice that the mean velocity $v \simeq \langle\dot{\theta}_1\rangle$, because $\langle\dot{\theta}_1\rangle \simeq \langle\dot{\theta}_2\rangle$.

At this point, what is left to do is to find the β integral as a function of the parameters in which we are interested. From now on, we will assume, for implicitly, that the energy is in $k_B T_1$ units. To simplify the calculation of the integral, we make an expansion of the denominator in Eq. (25) in powers of $\frac{1}{k}$. Since the value of k that we will consider is the one that makes the motor run faster ($k \simeq 100$), one can safely suppose that the terms of order $(\frac{1}{k})^2$ and so on will not notably contribute to the integral. Remember that d and V_0 are kept small. The relevant quantity β can then be written as

$$\beta = \int_0^L \mathrm{d}x \frac{\frac{1}{2}(-f(x)+\tau)(1 + \frac{f'(x)}{4k})}{\frac{1}{4}[1 + \frac{T_2}{T_1} + 2(1 - \frac{T_2}{T_1})\frac{f'(x)}{4k}]}. \tag{27}$$

Let us note that the terms $-f(x) + \tau$ in the numerator are very small when integrated. Therefore, we can neglect the much smaller correction $f'(x)/4k$ of the numerator. However, one cannot do this approximation for the same term in the denominator, because it is responsible for the net motion of the Brownian motor. Such a term contains two essential physical features. The first one is that it accounts for the multiplicative noise and thus, without it, thermal sources are unable to make the motor move. The second one is that it avoids the violation of the Second Law, i.e. when $T_2 = T_1$ it cancels and no average velocity is predicted. Then, the final and simplest expression for β is

$$\beta = 2\int_0^L \frac{-f(x) + \tau}{1 + \frac{T_2}{T_1} + 2(1 - \frac{T_2}{T_1})\frac{f'(x)}{4k}}\,\mathrm{d}x. \tag{28}$$

5. Simulations versus theory

Now that we have derived an analytical expression for the mean velocity of the motor, let us compare its predictions

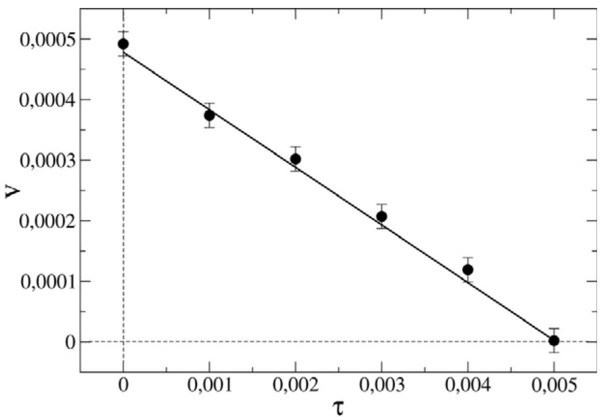

Fig. 5. Comparison between numerical simulations (dots) and theoretical prediction (line) from (33) of the dependence of the mean velocity v as a function of the external torque applied, τ. The parameters chosen are $k = 100$, $d = 4$, $V_0 = 3$ and $T_2 = 2T_1$.

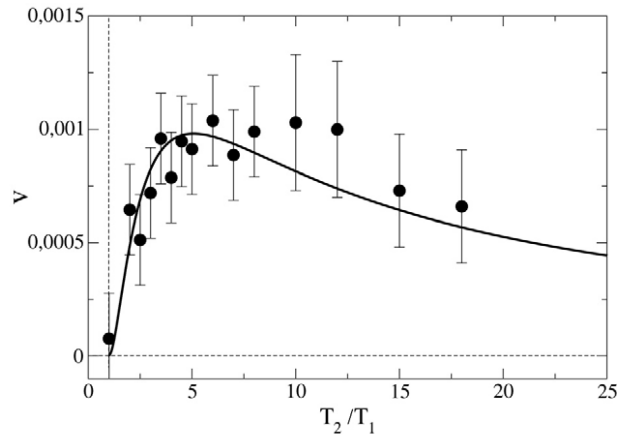

Fig. 6. Mean velocity v as a function of the ratio of temperatures T_2/T_1. The analytical prediction (line) fits the numerical results (dots) quite well, allowing for the fact that there is some uncertainty in the data obtained from the simulations. In this case, $\tau = 0$, and the other control parameters are unchanged.

with the numerical simulations when exploring two relevant parameters: the external torque τ and the temperature difference ratio T_2/T_1.

The first comparison is plotted in Fig. 5, in which we show the mean velocity as a function of the external torque. It is very remarkable that the stall torque (the torque at which the motor stops) is perfectly predicted by the expression found. What is more, the functional behavior (the linear dependence with negative slope) is clearly reproduced. To determine the scale, we adjust $\mathcal{N}$ so that the analytical prediction fits the simulations at $\tau = 0$, at the same time that we confirm that such a constant $\mathcal{N}$ does not depend very much on τ.

Since β is found to be very small, one can write the following expression for the mean velocity:

$$v = \mathcal{N}(1 - e^{\beta}) \simeq \mathcal{N}(-\beta) = a - \tau b, \tag{29}$$

where

$$a = 2\mathcal{N} \int_0^L \frac{f(x)}{1 + \frac{T_2}{T_1} + 2(1 - \frac{T_2}{T_1}) \frac{f'(x)}{4k}} \mathrm{d}x, \tag{30}$$

$$b = 2\mathcal{N} \int_0^L \frac{1}{1 + \frac{T_2}{T_1} + 2(1 - \frac{T_2}{T_1}) \frac{f'(x)}{4k}} \mathrm{d}x. \tag{31}$$

This last expression for the parameter b can be easily simplified by expanding its denominator and stopping at the first term, finding

$$b \simeq \frac{2\pi}{d} \frac{2\mathcal{N}}{1 + \frac{T_2}{T_1}}. \tag{32}$$

The term a is a little more complicated but it can be computed numerically. Finally, we obtain

$$v \simeq 0.00049 - 0.097\tau, \tag{33}$$

in units of s^{-1}. This result is plotted in Fig. 5.

Our second result is shown in Fig. 6, in which the prediction for the mean velocity is $v = a$, as one finds when setting $\tau = 0$ in Eq. (29). Despite data precision difficulties in the simulations, we can say that theory and simulations agree quantitatively and also reproduce three important qualitative facts. The first is that, at $T_1 = T_2$, the mean velocity is zero, as we explained before. The second is that there is a maximum of the speed (an optimal value for the ratio of temperatures). Third, we observe a slow decay of the velocity to zero as T_2 is increased. We also underline that the constant $\mathcal{N}$ used now is the same that we found for the $v(\tau)$ plot in Fig. 5. This again confirms our hypothesis that $\mathcal{N}$ depends very smoothly on the parameters that we are exploring (τ and T_2/T_1). When expanding the denominator of Eq. (30), we find that the terms appear as a function of the ratio T_2/T_1 and its powers. Therefore, we can roughly see that this more complex dependence of $v(T_2/T_1)$ comes from such terms. However, one must keep in mind that it is not a good idea to try to find exactly which these terms are, since our very first approximations killed terms of the same order in k. Nevertheless, we can say that our analytical predictions reproduce the numerical results very well. They capture the main qualitative behavior and also fit the quantitative data.

6. Conclusions

We have presented and studied a model for a thermal Brownian motor inspired by Feynman's ratchet and pawl [2]. After explaining Feynman's idea, we have introduced and justified the RPSBM model, and its main features have been explored numerically, finding the optimal regime of the motor. The results of the simulations are consistent with fundamental physical arguments that must always hold. We have performed an analytical calculation based on [5] with appropriate approximations to get an expression for the mean velocity in terms of the relevant parameters of the model. We have analyzed its dependence on the external torque τ and the ratio of temperatures T_2/T_1. Such formal predictions fit the data from the numerical simulations very well.

Regardless of the particular properties of these kinds of heat engines, they are in any case unrealistic models for molecular motors [16]. Firstly, it is known that such biological systems are mono-thermal and convert chemical energy into work, without the intermediate state of burning fuel. Secondly, the low efficiency of the engine leads us to discard the applicability of the model to biological motors. The mechanical coupling mechanism between both baths acts as a very good heat conductor, even in situations of very small mean velocity. Therefore, the efficiency is only a small fraction of that of Carnot. What is more, it is much smaller than the efficiency found in similar models [5], as one can see from the values of the velocity v. Such very low efficiency is a general feature of Brownian motors due to the fact that, in order to rectify thermal fluctuations, these systems must be tightly connected, and then a lot of heat is interchanged.

Acknowledgements

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