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Langevin model for a Brownian system with directed motion

Francisco Ambía and Humberto Híjar

Grupo de Sistemas Inteligentes, Facultad de Ingeniería, Universidad La Salle, Benjamín Franklin 47, 06140, Ciudad de México, México

E-mail: humberto.hijar@lasallistas.org.mx

Abstract. We propose a model for an active Brownian system that exhibits one-dimensional directed motion. This system consists of two Brownian spherical particles that interact through an elastic potential and have time-dependent radii. We suggest an algorithm by which the sizes of the particles can be varied, such that the center of mass of the system is able to move at an average constant speed in one direction. The dynamics of the system is studied theoretically using a Langevin model, as well as from Brownian Dynamics simulations.

1. Introduction

Understanding how a microscopic physical system is able to perform directed motion when it is immersed in an isotropic thermal bath, is a problem that has received considerable interest through the last decades [1, 2]. This interest has been increased by the observations of the mechanisms that allow molecular motors to perform specialized tasks in the cells of living organisms [3]. It is now known that such molecular machines use the spontaneous fluctuations occurring in their surroundings together with ratchet mechanisms, in order to break the spatial symmetry of their dynamics [4]. The understanding of such mechanisms could lead in the future to the fabrication of nanomachines aimed at functions such as targeted drug delivery, stirring and pumping in microfluidic devices, and separation of biological macromolecules [5]. Due to the significant impact that these applications would have, developing simplified models for the Brownian motors that retain the basic physical phenomena and can be mathematically treated, could be very helpful to understand the principles that govern their dynamics.

Directed Brownian motion can be achieved by employing a ratchet potential, i.e., a periodic potential with no reflection symmetry that is able to produce a net current of particles from unbiased thermal fluctuations [1]. In a more general context, a system is said to constitute a Brownian motor when [2]: the spatio-temporal periodicity critically affects the rectification mechanism, the averages of all acting forces and gradients vanish, random forces play a principal role, and it is kept in a nonequilibrium state by a rupture of the detailed balance symmetry. One-dimensional rectified Brownian motion appears in molecular transport through cell membranes, single-file diffusion, and noise-assisted transport promoted by oscillating barriers [6, 7, 8].

Here, we introduce a model for a one-dimensional Brownian motor which, to the best of our knowledge, has not been studied previously from the present point of view. Our main purpose is to study the dynamics of the proposed system analytically, by means of a Langevin model, and numerically by means of Brownian Dynamics (BD) simulations.

2. The model

Consider a system of two spherical particles restricted to move in one dimension. Let x_1 and x_2 denote the positions of these particles, and R_1 and R_2 their respective radii. It will be assumed that they interact through an elastic potential, $U = k (x_2 - x_1 - l)^2 / 2$, where k is the restoring coefficient and l is the equilibrium distance between the particles. The system will be immersed in a fluid with viscosity coefficient η . For mathematical simplicity, we will consider the mass of both particles to be equal to a constant m. R_1 and R_2 will be assumed to be sufficiently small such that the dynamics of the system can be well described by the over damped approximation. Using the center of mass position, $x_{c.m.} = (x_1 + x_2) / 2$, and the relative coordinate, $x_r = x_2 - x_1$, the dynamics of the system can be described in terms of the following system of Langevin equations

$$\frac{dx_{\text{c.m.}}}{dt} = -\frac{1}{2} \left(\frac{\omega^2}{\beta_2} - \frac{\omega^2}{\beta_1} \right) (x_{\text{r}} - l) + \frac{1}{2} \left(\frac{1}{\beta_1} \mathcal{A}_1 + \frac{1}{\beta_2} \mathcal{A}_2 \right),\tag{1}$$

$$\frac{dx_{\rm r}}{dt} = -\left(\frac{\omega^2}{\beta_1} + \frac{\omega^2}{\beta_2}\right)(x_{\rm r} - l) + \frac{1}{\beta_2}\mathcal{A}_2 - \frac{1}{\beta_1}\mathcal{A}_1,\tag{2}$$

where: $\omega = \sqrt{k/m}$; $\beta_i = aR_i/m$, with $a = 6\pi\eta$; and \mathcal{A}_i is the stochastic force per unit mass acting on the *i*th particle, for i = 1, 2.

As it is usual, stochastic forces will be considered as Markov-Gaussian processes with zero mean and fluctuation-dissipation theorem

$$\langle \mathcal{A}_{i}(t') \mathcal{A}_{j}(t) \rangle = \frac{2k_{B}T\beta_{i}}{m}\delta(t'-t)\delta_{ij}, \qquad (3)$$

where k_B is the Boltzmann constant, T is the temperature of the fluid, and no summation over repeated indices is implied.

If R_1 and R_2 are constants the formal solution of Eqs. (1) and (2) reads as

$$x_{\rm c.m.} = x_{\rm c.m.}^{o} + \tilde{\eta} \left(1 - e^{-\alpha t} \right) \left(x_{\rm r}^{o} - l \right) + \int_{0}^{t} d\xi \left[\psi_{\rm c.m.}^{(1)} \left(t - \xi \right) \mathcal{A}_{1} \left(\xi \right) + \psi_{\rm c.m.}^{(2)} \left(t - \xi \right) \mathcal{A}_{2} \left(\xi \right) \right], \quad (4)$$

$$x_{\rm r} = l + (x_{\rm r}^o - l) e^{-\alpha t} + \int_0^t d\xi \left[\psi_{\rm r}^{(1)} \left(t - \xi \right) \mathcal{A}_1 \left(\xi \right) + \psi_{\rm r}^{(2)} \left(t - \xi \right) \mathcal{A}_2 \left(\xi \right) \right].$$
(5)

In Eqs. (4) and (5), $x_{\text{c.m.}}^o$ and x_r^o are the initial values of the $x_{\text{c.m.}}$ and x_r , respectively; $\alpha = \omega^2 \left(\beta_1^{-1} + \beta_2^{-1}\right)$, is the characteristic inverse time for the damped dynamics of the system; and $\tilde{\eta} = (R_2 - R_1)/2(R_1 + R_2)$. The auxiliary functions $\psi_{\text{c.m.}}^{(i)}$, $\psi_r^{(i)}$, have the following definitions for i = 1, 2,

$$\psi_{\rm c.m.}^{(i)}(t) = \frac{m}{a} \left[\frac{e^{-\alpha t}}{2R_i} + \frac{1 - e^{-\alpha t}}{R_1 + R_2} \right], \ \psi_{\rm r}^{(i)}(t) = (-1)^i \frac{m}{a} \frac{e^{-\alpha t}}{R_i}.$$
(6)

3. Algorithm for directed motion

According to Eqs. (4) and (5), in the limit $t \gg \alpha^{-1}$, the average value of $x_r - l$ will vanish, while that of $x_{c.m.}$ will move by a total amount $\tilde{\eta} (x_r^o - l)$. Physically, this is a consequence of the fact that the bigger particle experiences a larger frictional force and acts as a kind of anchor for the coupled system, while the smaller is able to move due to the elastic interaction and drives the center of mass. As long as $x_r \neq l$, $x_{c.m.}$ will tend to move, on the average, in the direction determined by the sign of the product $\tilde{\eta} (x_r - l)$. Now, the perturbation brought about by the stochastic forces will drive x_r away from l persistently, and if $\tilde{\eta}$ could change its sign, due to a change in the values of R_1 and R_2 , then the product $\tilde{\eta} (x_r - l)$ might be forced to keep its sign constant, thus giving directed motion to the coupled system.

In the present work, we will explore the consequences of varying R_1 and R_2 between two defined values R_{max} and R_{min} ($R_{\text{max}} > R_{\text{min}}$), according to the following prescription

$$R_1 = R_{\max} \quad \text{and} \quad R_2 = R_{\min} \quad \text{if } x_r < l, R_1 = R_{\min} \quad \text{and} \quad R_2 = R_{\max} \quad \text{if } x_r > l.$$

$$(7)$$

Notice that when R_1 and R_2 are allowed to change in time according to the protocol Eq. (7), then Eqs. (4) and (5) are valid only for a short time interval, τ_1 , that lasts until the configuration of the system is updated. After that, the system evolves following similar equations but with modified functions such that $\tilde{\eta} \to -\tilde{\eta}$, $\psi_{\text{c.m.}}^{(1)} \to \psi_{\text{c.m.}}^{(2)}$, $\psi_{\text{c.m.}}^{(1)} \to \psi_{\text{c.m.}}^{(1)}$, $\psi_{\text{r}}^{(1)} \to -\psi_{\text{r}}^{(2)}$, and $\psi_{\text{r}}^{(2)} \to -\psi_{\text{r}}^{(1)}$. It can be shown from Eqs. (3) and (5), and from the previous symmetry properties, that the probability for observing an elongation of the system of magnitude \tilde{x}_{r} , at time t, given that it was \tilde{x}_{r}^{o} , at time zero, is the same as the one obtained for a system with fixed configuration.

On the other hand, in order to describe the statistical properties of $x_{c.m.}$, we will perform the following simplifying assumptions. First, that the stochastic processes of $x_{c.m.}$ during the time intervals of fixed configuration, τ_i , are statistically independent. Second, that the distribution of times τ_i has a small dispersion, in such a way that all configuration changes take place at regular time intervals with duration $\bar{\tau}$. Third, that observations of the system are performed after allowing the variable x_r to achieve its stationary distribution. Then, it can be shown that the probability for observing the center of mass at position $x_{c.m.}^{(n)}$, after *n* changes in configuration, given that its initial value was $x_{c.m.}^{(0)}$, is

$$W\left(x_{\rm c.m.}^{(n)}, n \,|\, x_{\rm c.m.}^{(0)}, 0\right) = \frac{1}{\sqrt{2\pi\sigma_n^2(\bar{\tau})}} \exp\left\{-\left[x_{\rm c.m.}^{(n)} - \left(x_{\rm c.m.}^{(0)} - \xi_n(\bar{\tau})\right)\right]^2 / 2\sigma_n^2(\bar{\tau})\right\},\tag{8}$$

where the functions $\sigma_n^2(\bar{\tau})$ and $\xi_n(\bar{\tau})$ are defined as $\sigma_n^2(\bar{\tau}) = n \left[\sigma_{\text{c.m.}}^2(\bar{\tau}) + (1 - e^{-\alpha\bar{\tau}})^2 \sigma_r^2\right]$, and $\xi_n(\bar{\tau}) = n \left(1 - e^{-\alpha\bar{\tau}}\right) |\tilde{\eta}| |\bar{x_r}|$ respectively.

In these definitions $\sigma_{\text{c.m.}}^2(\bar{\tau})$ represents the standard deviation for the distribution of $x_{\text{c.m.}}$ at time $\bar{\tau}$ which, for brevity, is not written explicitly; $\sigma_r^2 = k_B T/k$, is the stationary value of the corresponding standard deviation of x_r ; and $|\bar{x}_r| = \sigma_r \sqrt{2/\pi}$.

It can be shown that in the limit $\alpha \bar{\tau} \ll 1$, which can be achieved for large values of the k, we have $\sigma_n^2(\bar{\tau}) = n \bar{\tau} k_B T \left(R_{\min} + R_{\max} \right) / 2a R_{\min} R_{\max}$, and $\xi_n(\bar{\tau}) = v n \bar{\tau}$, where we have identified an average velocity for the Brownian motor as

$$v = \frac{1}{6\sqrt{2}\pi^{3/2}} \frac{R_{\max} - R_{\min}}{R_{\max}R_{\min}} \frac{\sqrt{kk_B T}}{\eta},$$
(9)

which as it could be expected increases with the radius difference, the thermal energy of the bath, and the strength of the elastic interaction, but decreases with the viscosity of the medium.

4. Comparison with Brownian Dynamics Simulations

We implemented BD simulations that allowed us to solve Eqs. (1) and (2), based on a Runge-Kutta-Maruyama scheme. In our implementation the units of length, mass and energy where fixed by the values $R_{\min} = 1$, m = 1, and $k_BT = 1$, respectively. We performed numerical experiments where the values of the restitution coefficient and the viscosity were fixed at $k = 5 k_B T/R_{\min}^2$, and $\eta = 5\sqrt{mk_B T}/R_{\min}^2$, respectively. Figure 1 *a*, shows the trajectories of five Brownian motors with different configurations characterized by the values of the percental radius difference, $\Delta = (R_{\text{max}} - R_{\text{min}})/R_{\text{min}} = 0.05, 0.10, 0.15, 0.20, 0.25$. It can be observed that the system exhibits, indeed, directed motion even for small values of Δ . The straight lines shown in Fig. 1 *a*, represent the corresponding motion at the constant speed given by Eq. (9). In Fig. 1 *a*, time is given in simulations units $(R_{\min}\sqrt{m/k_BT})$.



Figure 1. Comparison of the theoretical and numerical results. a Typical trajectories of Brownian motors with different configurations. Noise curves correspond with experimental results (symbols were included to guide the eye). b Standard deviation for the distribution function of the trajectory of two ensembles of Brownian motors with different configuration. Symbols represent numerical results and the continuous curves the analytical prediction.

We also conducted experiments where ensembles of 12500 independent Brownian motors were simulated. The standard deviation of the distribution of $x_{c.m.}^{(n)}$ for such ensembles was numerically calculated. Figure 1 *b* shows the results of such experiments for two different types of motors with configurations $\Delta = 0.05$ and 0.25. A comparison is performed with the standard deviation expected from the analytical model. A very good agreement of the theoretical and numerical approaches can be observed for small simulation times, while a deviation between them can be noticed for large values of *t*. This can be understood due to the simplifying assumptions used to obtain Eq. (8).

We notice that our model is similar to the so called *pushmepullyou* microswimmer introduced by Avron et al. in Ref. [9]. The main difference from that model and ours is that in Ref. [9] thermal forces were neglected while, here, they are the main mechanism that promotes the motion of the system. Extensions of the present work to include the effects of hydrodynamic fields around the Brownian motor similar to those considered in Refs. [9] and [10] are in progress.

References

- Hänggi P and Bartussek R 1996 Brownian rectifiers: how to convert Brownian motion into directed transport, in Nonlinear Physics of Complex Systems (Berlin: Springer) p 294
- [2] Hänggi P, Marchesoni F and Nori F 2005 Ann. Phys. (Leipzig) 14 51
- [3] Svoboda K, Schmidt C F, Schnapp B J and Block S M 1993 Nature 365 721
- [4] Hoffmann P M 2012 Life's Ratchet New York (Basic Books)
- [5] Leibler S 1994 Nature **370** 412
- [6] Bleil S, Reimann P and Bechinger C 2007 Phys. Rev. E 75 031117
- [7] Reichhardt C and Nori F 1999 Phys. Rev. Lett. 82 414
- [8] Speer D, Eichhorn R and Reimann P 2009 Phys. Rev. Lett. 102 124101
- [9] Avron J E, Kenneth O and Oaknin D H 2005 New J. Phys. 7 234
- [10] H. Híjar 2015 Phys. Rev. E 91 022139