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Hydrodynamic interactions induce movement against an external load in a ratchet dimer Brownian motor

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ABSTRACT

We use the Brownian dynamics with hydrodynamic interactions simulation in order to describe the movement of a elastically coupled dimer Brownian motor in a ratchet potential. The only external forces considered in our system were the load, the random thermal noise and an unbiased thermal fluctuation. For a given set of parameters we observe direct movement against the load force if hydrodynamic interactions were considered.

1. Introduction

Brownian motors are small physical micro- or even nano-machines that operate far from thermal equilibrium by extracting the energy from both, thermal and non-equilibrium fluctuations in order to generate work against external loads. They present the physical analogue of bio-molecular motors that also work out of equilibrium to direct intracellular transport and to control motion in cells. The most popular models assume an overdamped Brownian dynamics.

These molecular motors are powered by a ratchet mechanism, they convert the nonequilibrium fluctuation into directed flow of Brownian particles in an asymmetrical periodic potential (ratchet) without any net external force or bias. Several authors have studied theoretically the transport of two coupled particles modeling the two heads of a motor protein [1–6].

Nonequilibrium fluctuations, whether generated externally or by a chemical reaction far from equilibrium, can bias the Brownian motion of a particle in an anisotropic medium without thermal gradients, a net force such as gravity, or a macroscopic electric field. Fluctuation-driven transport is one mechanism by which chemical energy can directly drive the motion of particles and macromolecules and may find application in a wide variety of fields, including particle separation and the design of molecular motors and pumps.

In the present work we use the Brownian dynamics with hydrodynamic interactions simulation in order to describe the movement of a elastically coupled dimer Brownian motor in a ratchet potential.

In section entitled "The Model" we describe the forces acting on an oscillating dimer in a ratchet potential with a load force and an external unbiased fluctuation, which acts simultaneously on two particles. In section "Hydrodynamic Interactions" we describe the origin of this interactions in the low Reynolds number limit till the definition of the Diffusion tensor. In the section untitled "Brownian dynamics with hydrodynamic interactions" we describe the formalism given by Ermak and McCammon [10], which couples the forces described in "The Model" section and thermal noise with the Diffusion tensor.

2. The Model

We consider an elastically coupled dimer in three dimensions in an asymmetrical potential (ratchet) in the x direction, see Fig. 1, namely [7],

$$U_{rat}(x_i) = \frac{1}{2\pi}\left[\sin\left(\frac{2\pi x_i}{L}\right) + \frac{1}{4}\sin\left(\frac{4\pi x_i}{L}\right)\right] \tag{1}$$

The corresponding force on the particles produced by the ratchet potential is given by:

$$F_{rat}(x_i) = -\frac{\partial U_{rat}(x_i)}{\partial x_i} = -\frac{1}{L}\left[\cos\left(\frac{2\pi x_i}{L}\right) + \frac{1}{2}\cos\left(\frac{4\pi x_i}{L}\right)\right] \tag{2}$$

In the former equations x_i is the x coordinate of particle i, $i = 1$ and 2, to distinguish the dimer particles.

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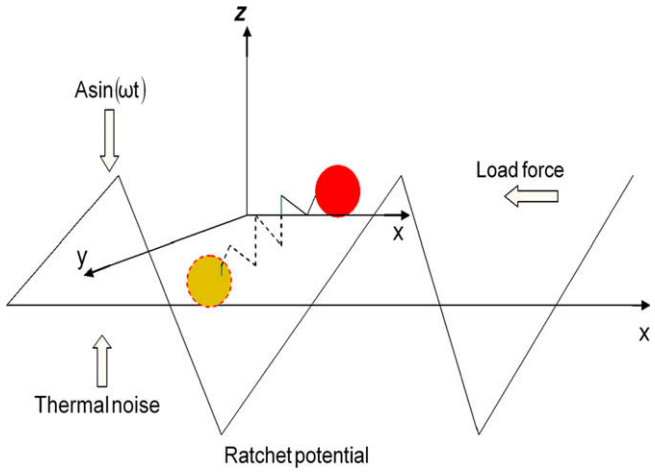

Fig. 1. Dimer in a ratchet potential.

We define $\mathbf{r_{ij}}$ the vector from the center of particle i to the center of particle j, for particles $i = 1$, $j = 2$, we have

$$\mathbf{r}_{12} = x_{12}\mathbf{i} + y_{12}\mathbf{j} + z_{12}\mathbf{k} \tag{3}$$

i, **j**, **k** are unit vectors in the direction of the cartesian axis, with

$$\begin{aligned} x_{12} &= x_1 - x_2 \\ y_{12} &= y_1 - y_2 \\ z_{12} &= z_1 - z_2 \\ r_{12} &= \left(x_{12}^2 + y_{12}^2 + z_{12}^2\right)^{1/2} \end{aligned} \tag{4}$$

Then the modulus of the harmonic force is,

$$F_{12} = |k(l_0 - r_{12})| \tag{5}$$

where k is the strength of the harmonic potential and l_0 is the equilibrium position.

Then the components of the harmonic force are,

$$\begin{aligned} F_{x_{12}} &= F_{12}\frac{x_{12}}{r_{12}} \\ F_{y_{12}} &= F_{12}\frac{y_{12}}{r_{12}} \\ F_{z_{12}} &= F_{12}\frac{z_{12}}{r_{12}} \end{aligned} \tag{6}$$

The corresponding components of the harmonic force on each dimer particle are,

$$\begin{aligned} F_{har}(x_1) &= F_{12}\frac{x_{12}}{r_{12}} = -F_{har}(x_2) \\ F_{har}(y_1) &= F_{12}\frac{y_{12}}{r_{12}} = -F_{har}(y_2) \\ F_{har}(z_1) &= F_{12}\frac{z_{12}}{r_{12}} = -F_{har}(z_2) \end{aligned} \tag{7}$$

Then the forces acting on the dimer particles are:

$$\begin{aligned} F_{x1} &= F_{har}(x_1) + F_{rat}(x_1) - F_{load} + \varepsilon_x(t) \\ F_{y1} &= F_{har}(y_1) \\ F_{z1} &= F_{har}(z_1) \\ F_{x2} &= -F_{har}(x_1) + F_{rat}(x_2) - F_{load} + \varepsilon_x(t) \\ F_{y2} &= -F_{har}(y_1) \\ F_{z2} &= -F_{har}(z_1) \end{aligned} \tag{8}$$

The load force, F_{load}, acts to oppose the motor's forward progress, $\varepsilon_x(t) = A\sin(\omega t)$ is an external unbiased fluctuation, which acts simultaneously on two particles.

3. Hydrodynamic interactions

Consider a particle embedded in a viscous liquid, the movement of the surrounding incompressible fluid at the regime of Stokes-flow (low Reynolds number $\mathrm{Re} = \frac{d\rho}{\eta}\mathrm{v}$) is governed by

$$\nabla p - \eta\nabla^2\mathbf{v} = \mathbf{f}(\mathbf{r}) \tag{9}$$

$$\nabla\mathbf{v} = 0 \tag{10}$$

where d is the size of the system ρ and η are the density and the viscosity of the fluid respectively, $\mathbf{v}$ is the velocity field, see Fig. 2, $p(\mathbf{r})$is the local pressure and $\mathbf{f}(\mathbf{r})$is the force density.

The general solution of these inhomogeneous linear equations is given by the super-position of a solution of the homogeneous equation, $\mathbf{v}_{ext}(\mathbf{r})$, which is the externally imposed flow field, and a special solution

$$\mathbf{v}_{ind} = \int d\mathbf{r}'\mathcal{O}(\mathbf{r},\mathbf{r}')\mathbf{f}(\mathbf{r}') \tag{11}$$

of the inhomogeneous equation. The Green's function of Eq. (11) is called the Oseen-tensor $\mathcal{O}(\mathbf{r},\mathbf{r}')$, its Cartesian matrix elements are given by [8,9]

$$\mathcal{O}_{ij}(\mathbf{r},\mathbf{r}') \equiv \frac{1}{8\pi\eta|\mathbf{r}-\mathbf{r}'|}\left[\delta_{ij} + \frac{\left(r_i - r_i'\right)\left(r_j - r_j'\right)}{|\mathbf{r}-\mathbf{r}'|^2}\right] \tag{12}$$

Thus, the hydrodynamics mediates a long-range interactions ($\backsim 1/|\mathbf{r}\text{-}\mathbf{r}'|$) between the force $\mathbf{f}$ acting at $\mathbf{r}'$ and the velocity $\mathbf{v}$ induced at $\mathbf{r}$. The total velocity field becomes

$$\mathbf{v}(\mathbf{r}) = \mathbf{v}_{ext}(\mathbf{r}) + \mathbf{v}_{ind}(\mathbf{r}) \tag{13}$$

The relation between the Diffusion, D, and Oseen, $\mathcal{O}$, tensors is given by

$$D_{ij} = D_0\delta_{ij}I + \left(1 - \delta_{ij}\right)k_BT\mathcal{O}_{ij} \tag{14}$$

$D_0 = k_BT/6\pi\eta a$ is the diffusion coefficient of a single subunit sphere, δ_{ij} is the Kronecker delta, I is the unit tensor and a is the particle radius. Eq. (14) can be split in two, namely

$$\begin{aligned} D_{ij} &= D_0\delta_{ij}, i,j \quad \text{on the same particle} \\ D_{ij} &= \frac{3}{4}D_0\frac{a}{r_{ij}}\left(I + \frac{\vec{r_{ij}}\otimes\vec{r_{ij}}}{r_{ij}^2}\right), i,j \quad \text{on different particles} \end{aligned} \tag{15}$$

$\vec{r_{ij}}\otimes\vec{r_{ij}}$ is the dyadic product, for particles $i = 1$, $j = 2$, we have

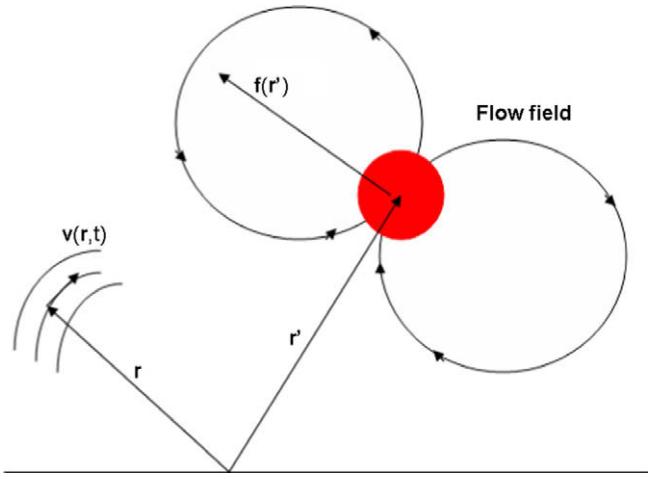

Fig. 2. The particle at $\mathbf{r}'$ exerts a force $f(\mathbf{r}')$ onto the liquid which affects the velocity $\mathbf{v}(\mathbf{r})$.

$$\vec{r_{12}} \otimes \vec{r_{12}} = \begin{bmatrix} x_{12} \\ y_{12} \\ z_{12} \end{bmatrix} [x_{12}\ y_{12}\ z_{12}] = \begin{bmatrix} x_{12}^2 & x_{12}y_{12} & x_{12}z_{12} \\ y_{12}x_{12} & y_{12}^2 & y_{12}z_{12} \\ z_{12}x_{12} & z_{12}y_{12} & z_{12}^2 \end{bmatrix} \tag{16}$$

As an example we show the Diffusion tensor for two particles in a two dimensional system,

$$D = D_0 \begin{bmatrix} 1 & 0 & \frac{3}{4}\frac{a}{r_{12}}\left(1+\frac{x_{12}^2}{r_{12}^2}\right) & \frac{3}{4}\frac{a}{r_{12}}\frac{x_{12}y_{12}}{r_{12}^2} \\ 0 & 1 & \frac{3}{4}\frac{a}{r_{12}}\frac{x_{12}y_{12}}{r_{12}^2} & \frac{3}{4}\frac{a}{r_{12}}\left(1+\frac{y_{12}^2}{r_{12}^2}\right) \\ \frac{3}{4}\frac{a}{r_{12}}\left(1+\frac{x_{12}^2}{r_{12}^2}\right) & \frac{3}{4}\frac{a}{r_{12}}\frac{x_{12}y_{12}}{r_{12}^2} & 1 & 0 \\ \frac{3}{4}\frac{a}{r_{12}}\frac{x_{12}y_{12}}{r_{12}^2} & \frac{3}{4}\frac{a}{r_{12}}\left(1+\frac{y_{12}^2}{r_{12}^2}\right) & 0 & 1 \end{bmatrix} \tag{17}$$

4. Brownian dynamics with hydrodynamic interactions

Consider a system of N spherical interacting Brownian particles suspended in a hydrodynamic medium, the displacement of particle i during $\triangle t$ is given by Ermak and McCammon [10], namely

$$r_i = r_i^0 + \sum_j \frac{D_{ij}^0 F_j^0}{k_B T} \triangle t + R_i(\triangle t) \tag{18}$$

where the superscript "0" indicates that the variable is to be evaluated at the beginning of the time step. F_j^0 is the force acting on particle j. $R_i(\triangle t)$ is a random displacement with a Gaussian distribution function whose average value is zero and the correlation is $\langle R_i(\triangle t) R_j(\triangle t)\rangle = 2D_{ij}^0 \triangle t$.

5. Results and conclusions

All of the results are expressed in dimensionless units. Distance is in units of the separation distance l_0 and time is in units of l_0^2/D_0. We used in the simulations the following parameters: $l_0 = 1$, $L = 1$, $k = 100$, $a = 0.1$, $D_0 = 1$, $\triangle t = 0.00125$, the simulation time was $t = 1125$, which corresponds to 9×10^5 steps.

The average center of mass velocity in the x direction, $\langle v_{cx}\rangle$, in the long-time limit, i.e., after transients due to initial conditions have died out, is given by

$$\langle v_{cx}\rangle = \langle \dot{x}_c(t)\rangle_{st} = \lim_{t\to\infty} \frac{\langle x_c(t)\rangle - \langle x_c(0)\rangle}{t} \tag{19}$$

where $x_c(t) = [x_1(t) + x_2(t)]/2$ and the mean $\langle v_{cx}\rangle$ is on the realizations of the stochastic process.

Each point of the curves of Figs. 3 and 5 is the result of 100 stochastic realizations. At the stationary state, the ratio $SE\ (\langle v_{cx}\rangle)/\langle v_{cx}\rangle \leqslant 10^{-3}$, where $SE\ (\langle v_{cx}\rangle)$ is the standard error of the mean velocity $\langle v_{cx}\rangle$.

The average velocity of a molecular motor is a function of the load force resisting the motor's advancement. One of the characteristic of a molecular motor is the load force–velocity curve. In Fig. 3 we show $\langle v_{cx}\rangle$ as a function of the load force F_{load}, for the case $A = 0$, without the external unbiased fluctuation.

We were able to find a set of parameters in which the effect of hydrodynamic interactions is shown.

In the range $-5 \leqslant F_{load} \leqslant 0$ and only in the case with hydrodynamic interactions, we observe, the motor continue with a positive velocity in spite of the negative load force (ratchet effect).

In the case without hydrodynamic interactions the motor is dragged along by the load force and the velocity has the same sign of the load force.

In Fig. 4 we observe the behaviour of the average center of mass velocity in the x direction, $\langle v_{cx}\rangle$, in the long-time limit, i.e., after

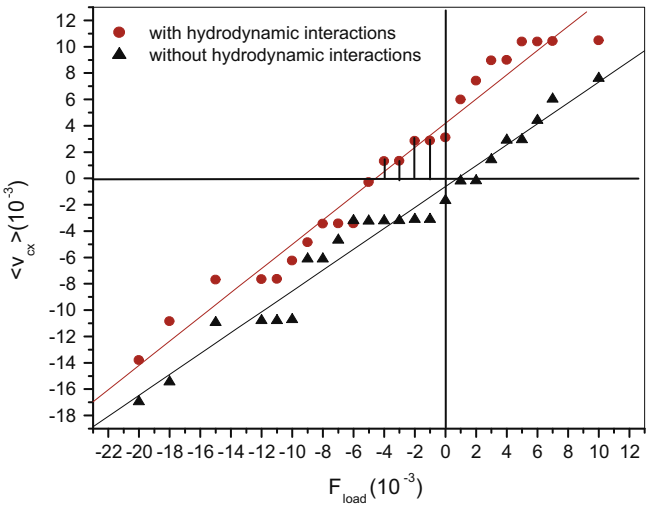

Fig. 3. $\langle v_{cx}\rangle$ vs. F_{load} for the case $A = 0$, Linear fitting $R = 0.98$, $P < 0.001$ in both curves, $l_0 = 1$, $L = 1$, $k = 100$, $a = 0.1$, $D_0 = 1$.

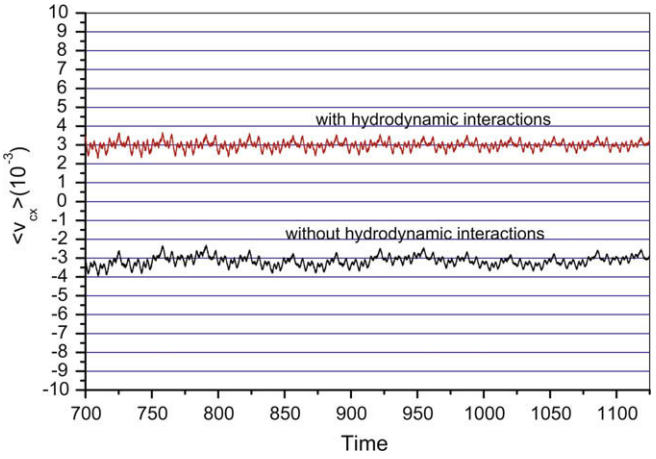

Fig. 4. $\langle v_{cx}\rangle$ vs. *time* in the long time limit for the case $A = 0.$, $l_0 = 1$, $L = 1$, $k = 100$, $a = 0.1$, $D_0 = 1$, $F_{load} = -0.002$.

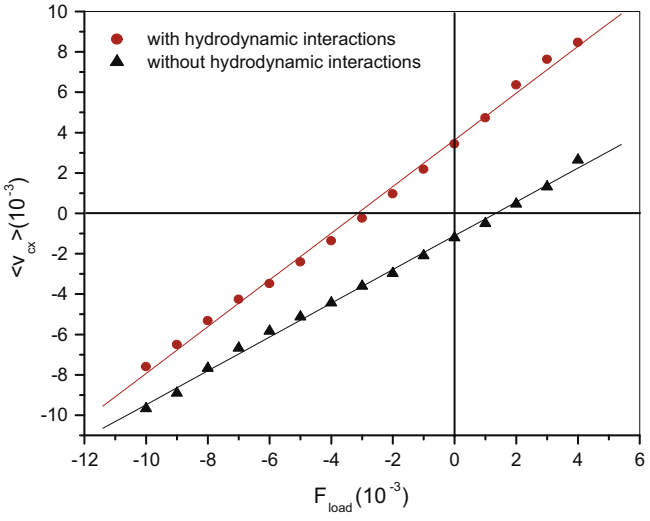

Fig. 5. $\langle v_{cx}\rangle$ vs. F_{load} for the case $A = 0.1$, linear fitting $R = 0.99$, $P < 0.001$ in both curves, l_0=1, $L = 1$, $k = 100$, $a = 0.1$, $D_0 = 1$, $A = 0.1$, $\omega = 1$.

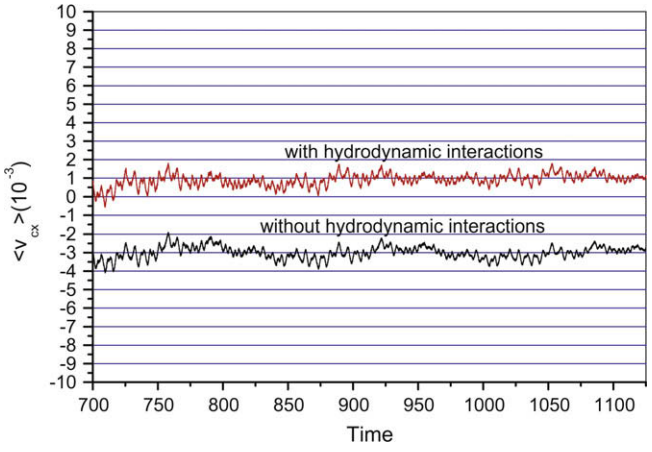

Fig. 6. $\langle v_{cx} \rangle$ vs. *time* in the long time limit for the case $A = 0.1$, $\omega = 1$, $l_0 = 1$, $L = 1$, $k = 100$, $a = 0.1$, $D_0 = 1$, $F_{load} = -0.002$.

transients due to initial conditions have died out for a given load force for the case $A = 0$. The velocity is substantially greater for the case with hydrodynamic interactions.

In this case the fluctuations are only thermal, 3rd right hand side term of Eq. (18). These thermal fluctuations excite the oscillating modes of the dimer, as a consequence, the imposed external ratchet potential has an oscillatory unbiased component, this would be the driving force. Indeed this is the conversion (or rectification) of random fluctuations into useful work and is termed the "ratchet effect".

In Fig. 5 we show $\langle v_{cx} \rangle$ as a function of the load force F_{load}, for the case $A = 0.1$, $\omega = 1$, with the external unbiased fluctuation. In contrast with the case $A = 0$. we observe almost a perfect linear curve although the result is similar, namely the hydrodynamic interaction increase the dimer movement. For high values of A, the hydrodynamic interaction effect could be masked. In Fig. 6 we observe the behaviour of the average center of mass velocity in the x direction, $\langle v_{cx} \rangle$ in the long time limit, for the case $A = 0.1$, $\omega = 1$, with the external unbiased fluctuation. We also observe an increase in $\langle v_{cx} \rangle$ when hydrodynamic interactions are considered.

A similar result was found by Houtman et al. [11] who developed a simple 2D-lattice model in order to test the influence of hydrodynamic interactions on the collective transport of molecular motors, which is important for the understanding of cell growth and development. Houtman et al. shown that long range collective hydrodynamic interactions lead to a substantial increase in the effective velocity of motors attached to a filament. Their results were also supported by experiments.

In conclusion hydrodynamic interactions influence substantially the behaviour of a dimer molecular motor, consequently they have to be considered in any theory where the molecular motors are in a liquid medium.

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