Brownian motors in variable shape potential: overdamped versus underdamped

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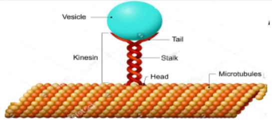
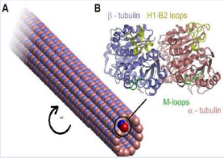
- Definition of Brownians Motors;
  - transport properties across biology membranes,
  - superionic conductors,weakly pinned charged-density-wave condensates,
  - submonolayer films adsorbed on crystalline substrate,
  - Josephson junctions,
- To study the diffusion mechanism of mobile particles through the ionic solids, we suppose that they are as system of $\mathbb{N}$ Brownian particles submerged in a periodic potential,
- The deformed substrate can represent a substrat which have abnormalities and defects, conformational changes;

(a) 

(b) 

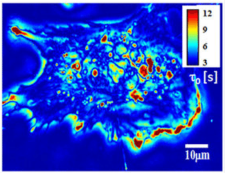
(c) 

Figure: (a) Diagram illustrating motility of kinesin, (b) Microtubules and the crystallographic structure of the human kinesin motor.

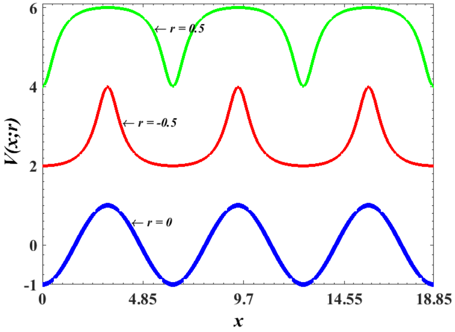
The environment are well described by the following Langevin equation

$$m\ddot{x} + \gamma \dot{x} = -\frac{dV(x,t;r)}{dx} + \sqrt{2\gamma K_B T}\varepsilon(t), \qquad (1)$$

- m represents the mass of the Brownian particle,
- γ is the friction coefficient,
- The zero-mean and the δ-correlated Gaussian white noise, $\varepsilon(t)$, meaning that $< \varepsilon(t)\varepsilon(s) >$ = $\delta(t-s)$, models the influence of the temperature T on the system
- $D = \gamma KT$, where K is the Boltzmann constant represents the diffusion coefficient also known as the noise intensity,

- $V(x,t;r) = \left(\frac{(1+r)^2(1-\cos(x-\omega t))}{(1-r)^2 + 2r(1-\cos(x-\omega t))} - 1 \right)$
- ω represents the travelling potential

- $|r| < 1$ represents the deformation parameter,
- $r = 0$, the potential reduces to a sinusoidal shape,
- $r < 0$ it provides broad wells separated by narrow barriers,
- $r > 0$ it provides deep narrow wells separated by broad flat barriers



The dynamic of system is described by the corresponding Fokker-Planck equation

$$\frac{\partial}{\partial t}P(x,v,t) = L_F P(x,v,t), \tag{2}$$

where

$$L_F = -v\frac{\partial}{\partial x} + \left(\frac{\partial}{\partial v}\right)\left(V'(x,t;r) + \gamma v\right) + D^2\frac{\partial^2}{\partial v^2}. \tag{3}$$

Overdamped case ($m = 0$)

- Model the orientation of molecular motor's internal electric dipole in order to describe the nature of interaction between the motor and the filaments;
- Applying the following periodic boundary condition and normalization condition,
  - $P(x + 2\pi, t) = P(x, t)$,
  - $\int_0^{2\pi} P(x, t) = 1$,

$$P(x - \omega t) = \frac{1}{Z} \int_0^{2\pi} d\alpha \exp\left(\frac{V(x + \alpha - \omega t; r) - V(x - \omega t; r) + \omega\alpha}{D} \right), \tag{4}$$

$$< v > = \omega + 2\pi C, \tag{5}$$

$$C = \frac{D\left(1 - \exp(\frac{2\pi\omega}{D})\right)}{Z}, \tag{6}$$

$$Z = \int_0^{2\pi} d\alpha \int_0^{2\pi} dx \exp\left(\frac{V(x+\alpha; r) - V(x; r) + \alpha\omega}{D}\right). \tag{7}$$

Underdamped case ($m \neq 0$)

- Driven plasma waves, known to accelerate classical charged particles trapped by a perpendicular propagating electrostatic waves

$$P(x, v, t) = \sum_{n=0}^{\infty} C_n(x, t)\psi_n(v), \tag{8}$$

$C_n(x, t)$, are the expansion coefficients and $\psi_n(v)$, the hermite function. Where

$$\frac{\partial \mathbf{C}}{\partial t} = -\alpha \mathbf{R} \frac{\partial \mathbf{C}}{\partial x} + \mathbf{SC}, \tag{9}$$

where **R** and **S** are $(N+1)\times(N+1)$ matrices given by

$$\mathbf{R} = \begin{pmatrix} 0 & \alpha_1 & & & \\ \alpha_1 & 0 & \alpha_2 & & \\ & \ddots & \ddots & \ddots & \\ & & \alpha_N & & \alpha_N \end{pmatrix} \tag{10}$$

and

$$\mathbf{S} = \begin{pmatrix} 0 & 0 & \cdots & 0 & \cdots \\ -\frac{\sqrt{2}}{\alpha}A & -\gamma & 0 & \cdots & \\ 0 & -\frac{2}{\alpha}A & -2\gamma & 0 & \cdots \\ 0 & 0 & -\frac{\sqrt{6}}{\alpha}A & -3\gamma & \cdots \\ \vdots & \ddots & \ddots & \ddots & \ddots \end{pmatrix} \tag{11}$$

with $A = V'(x,t;r)$ and where $\alpha_n = \sqrt{n/2}$.

- For the numerical treatment in both cases, the average velocity, the effective diffusion and the monte carlo error of Eq.(1), are respectively given by

$$\langle v \rangle = \lim_{t \to \infty} \frac{\langle x(t) \rangle}{t}, \tag{12}$$

$$D_{eff} = \lim_{t \to \infty} \frac{\left\langle x(t)^2 \right\rangle - \langle x(t) \rangle^2}{2t}, \tag{13}$$

$$\sigma = \frac{1}{\sqrt{L}} \sqrt{\left\langle v^2 \right\rangle - \langle v \rangle^2}. \tag{14}$$

overdamped case ($m = 0$)

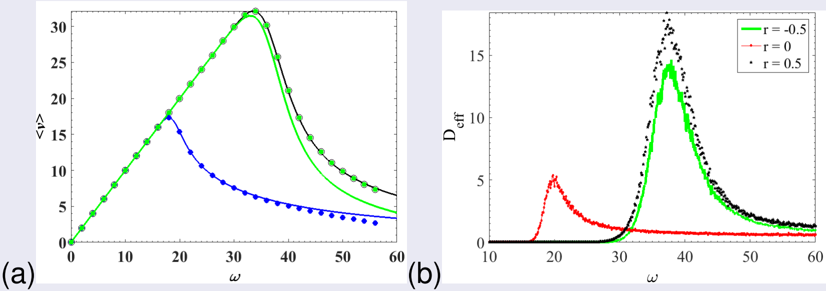


Figure: (a) Average velocity of Brownian particles and the analytical result for r=0,-0.5,0.5 as a function of the travelling potential ω, (b) Schematic representation of effective diffusion of Brownian particle in the overdamped regime as a function of the travelling speed ω for few values of r.

Numerical result

(c)

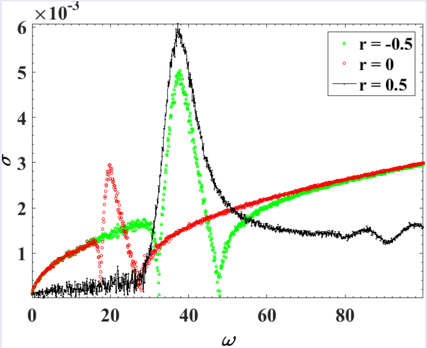
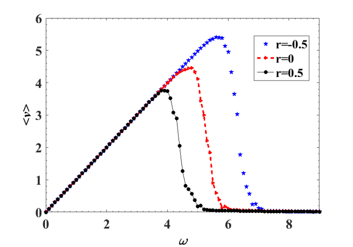


Figure: Monte Carlo error σ vs ω for different values of the shape parameter r.

underdamped case ($m \neq 0$)

(a) 

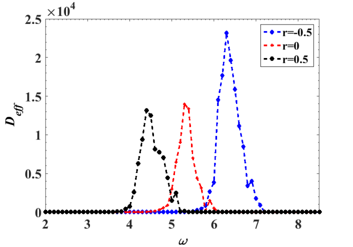
(b) 

Figure: (a)Representation of average velocity as a function of ω for different values of the shape parameter r in underdamped case, (b) plot of the effective diffusion D_{eff} as a function of the travelling potential speed ω for some values of shape parameter r ($r = -0.5$, $r = 0$, $r = -0.5$).

underdamped case ($m \neq 0$)

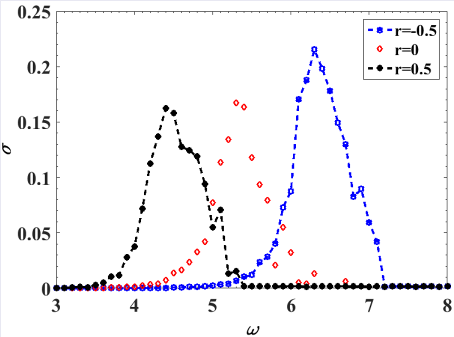


Figure: Monte Carlo error representation of underdamped case

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underdamped case ($m \neq 0$)

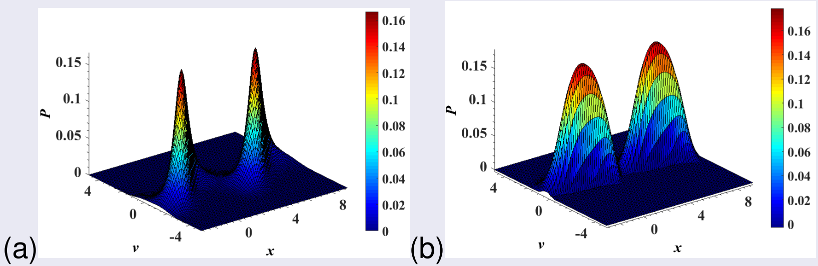


Figure: (a)Distribution of the Brownian particle in deformable potential for $r = 0$ at $t = 1$, (b) Distribution of the Brownian particle in deformable potential for $r = -0.5$ at $t = 2$.

underdamped case ($m \neq 0$)

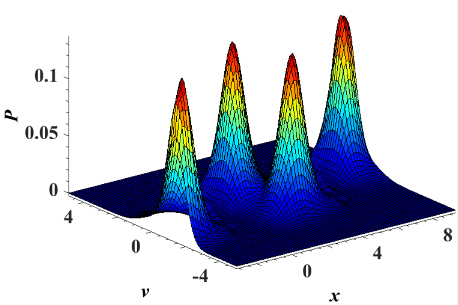
(c) 

Figure: (c) Distribution of the Brownian particle in deformable potential for $r = 0.5$ at $t = 2$. This case tends to split in several modes.

- We show in both cases that the critical value of the travelling potential speed ω for which the average velocity of the Brownian motor is maximal, where unpinning occurs, depends on the intensity of the noise, as previously shown, but we find it is also a function of the shape.
- In underdamped case, one note a giant enhancement diffusion with respect to the overdamped case.
- For some shapes of the system, the distribution may exhibit several modes.
- Globally, biological systems are soft matter and their shape and conformation may change due to external effects. Thus modelling such systems it is necessary to take into account their geometry.

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