SYMMETRY BASED MODELING THE FUNCTIONING OF POLAR BROWNIAN ROTOR

Nastassia Savina, Irina Shapochkina

Department of Physics, Belarusian State University, Belarus
sadfiz@mail.ru

This work is devoted to the theoretical analysis of Brownian motors (ratchets), which are the systems that can demonstrate directional motion of nanoparticles as a result of rectification of nonequilibrium unbiased fluctuations of various nature in the absence of static forces and concentration gradients [1]. This effect is observed in a large variety of biological and artificial systems [2]. Molecular Brownian rotors (rotating Brownian ratchets) can manifest repetitive unidirectional rotational movement.

Our study is based on the description presented in [3], where the theory of the azimuthal jumping motion of an adsorbed polar molecule in a periodic *n*-well potential has been developed. It was shown that, for a symmetric potential of hindered rotation, unidirectional rotation a Brownian dipole rotator is possible only at both n=2 and simultaneous modulation of the minima and maxima of the potential by an external alternating electric field.

Our aim was to study the influence of temperature, fluctuation frequency and symmetries of the spatial and temporal dependences of the particle potential energy on the behavior of the average angular velocity of Brownian dipole rotator with the potential energy of the following form [4]:

$$U(\varphi,t) = \frac{1}{2}u[1 - cos2(\varphi - \Phi)] - \mu E(t)\cos(\varphi - \varphi_0) \quad (1)$$

Here μ is the rotor dipole moment, u is the barrier of the hindered rotation, Φ and φ_0 are the phase shifts of the stationary and fluctuating parts of the potential.

System (1) is an example of a ratchet system with an additive-multiplicative form of the particle potential energy,

$$U(x,t) = u(x) + \sigma(t)w(x), \quad (2)$$

(if we put $\varphi = 2\pi x/L$, $\Phi = 2\pi\lambda$, and $\varphi_0 = 2\pi\lambda_0$) for which a number of effective theoretical approaches are developed [6]. In the high-temperature approximation, the average Brownian rotor velocity is calculated as [4,5]:

$$\langle v\rangle = k_1 D\widetilde{\psi_2}\beta^3 w^2 \frac{u}{4}\sin 4\pi(\lambda - \lambda_0) \quad (3)$$

where k_1 is the wave number, D is the diffusion coefficient, β is the inverse thermal energy, $\widetilde{\psi_2} \equiv Dk_1^2\psi_2(Dk_1^2, Dk_1^2)$ is the dimensionless function (Eq. (15) in [4]), w is the amplitude of $w(x)$.

Symmetry-conditioned effects were analyzed within the approach suggested in [7], which showed that for a system (2) with a-symmetric forces $f(x) = -u'(x)$, $g(x) = -w'(x)$, with symmetry centers $x_a^{(f)}$ and $x_a^{(g)}$, respectively, $f\left(x + x_a^{(f)}\right) = -f(-x+x_a^{(f)})$ and $g\left(x + x_a^{(g)}\right) = -g(-x+x_a^{(g)})$, the following property takes place [7]:

$$v\{f_a(x) + g_a(x)\sigma(t)\} = -v\left\{ f_a\left(x + 2x_a^{(f)} - 2x_a^{(g)}\right) + g_a(x)\sigma(t)\right\} \quad (4)$$

Thus, at $x_a^{(f)} \neq x_a^{(g)}$, the total force is not a-symmetric, and, hence, the ratchet effect may exist even for symmetric $u(x)$ and $w(x)$. This approach was used for analyzing the high-temperature Brownian rotor with the potential energy (1). The results were compared with the analysis in [3] and [5].

Theoretical analysis outside the high-temperature approximation required numerical solution of equations for the Green function of diffusion in the stationary part of the potential profile [6], $u(x)$, and numerical calculating of a double integral.

The frequency and temperature dependencies of the average rotor velocity have been obtained and interpreted, as well as the influence of the geometrical parameters of the system on the regime of particle motion (in particular, on existence of stopping points) has been studied. Symmetry analysis yielded conclusions on the orientations of the external electric field permitted for the appearance of directed rotation.

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