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Diffusion Study of Coupled Brownian Ratchet

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Abstract: In this paper, the effective diffusion coefficient of the coupled Brownian ratchet is studied. Langevin equation is used to describe the coupled Brownian ratchet model, and the Runge-Kutta algorithm is used to solve the equation. The average velocity of the coupled Brownian particle is obtained, and the effective diffusion coefficient of the coupled ratchet is further calculated. The numerical calculation method of the effective diffusion coefficient of coupled Brownian particles has been widely used in many research fields. By using this numerical strategy, researchers can deeply understand the dynamic behavior of complex systems and provide theoretical support for the research and application in related fields.

Keywords: Coupled Brownian ratchet; Average velocity; Effective diffusion coefficient; Runge-Kutta algorithm

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1. Introduction

Biomolecular motors, as a kind of important nanoscale molecular machines, are mainly composed of proteins and nucleic acids and widely exist in all kinds of cells. This kind of motor obtains chemical energy by hydrolyzing ATP or uses electrochemical potential generated by transmembrane proton gradient as a power source [1]. Different from macroscopic artificial motors, molecular motors operate in a solution environment with low Reynolds number and high viscosity, their motion characteristics are subject to overdamping conditions, and they cannot rely on inertia to maintain the motion state [2]. Molecular motors play an indispensable role in the activities of life, from muscle contraction and intracellular material transport to DNA replication and cell division, and other processes rely on hundreds of molecular motors working together. These nanomachines can actively take up ATP molecules in the environment, use the energy generated by their hydrolysis, and achieve directional motion in response to thermal fluctuations [3].

To further explore the directional transport mechanism of molecular motors, researchers built a Brownian ratchet model based on Brownian motion theory [4]. The essence of this model is to realize directional transport by breaking the thermodynamic equilibrium state of the system and destroying the spatial symmetry [5]. According to the different ways of non-equilibrium driving, Brownian ratchet models can be divided into four categories:

(1) rocking ratchet models, which are characterized by the disturbance of thermal balance by unbiased external forces, resulting in directional motion in asymmetric potential fields [6–7]; (2) the scintillation ratchet model, whose mechanism results from the random switching or periodic modulation of the asymmetric potential field between multiple states [8–9]; (3) the correlated ratchet model, whose directional transport is triggered by time correlation effects or spontaneous collective motion [10–11]; (4) self-driven ratchet model, which is characterized by breaking the thermal balance through self-driving force and achieving net transport in an asymmetric structure [12–13]. In recent years, the research on directional transport of Brown ratchet has made remarkable progress. For example, Li et al. revealed the reversal of the direction of motion of collective directional transport in coupled systems and found that the reversal of the direction of motion can be achieved by adjusting the coupling strength, free length, and potential field asymmetry coefficient [14]. Xu et al. found that the ratchet effect of overdamped Brownian particles is suppressed by increasing the noise intensity in a spatially symmetric potential field [15]. In this paper, the characteristics of the centroid diffusion coefficient (Deff) of the coupled Brownian ratchet are discussed, and its calculation method is deeply analyzed.

2. The theoretical research of coupled Brownian ratchet

In this paper, the diffusion of coupled Brownian particles is studied. The motion of two coupled Brownian particles is described by the Langevin equation as follows.

$$\dot{x}_1(t) = -\frac{\partial U(x_1)}{\partial x_1} - \frac{\partial F(x_1,x_2)}{\partial x_1} + \xi_1(t), \quad (1)$$

$$\dot{x}_2(t) = -\frac{\partial U(x_2)}{\partial x_2} - \frac{\partial F(x_1,x_2)}{\partial x_2} + \xi_2(t), \quad (2)$$

In the above formula (1) and (2), x_1(t) and x_2(t) respectively represent the position of the two coupled particles at the moment), U(x) is the asymmetric periodic external potential, F(x1, x2) representing the interaction potential between the two coupled Brownian particles, the specific form is as follows:

$$F(x_1, x_2) = \frac{1}{2}k(x_1 - x_2 - a)^2, \quad (3)$$

1(t) and ξ2(t) are Gaussian white noise and satisfies the following properties

$$\langle \xi_i(t) \rangle = 0, \quad (4)$$

$$\langle \xi_i(t)\xi_j(t') \rangle = 2D\delta_{ij}\delta(t - t'), i, j = 1,2. \quad (5)$$

In the formula (5), D represents the thermal noise intensity, its value is k_BT_0, k_B represents the Boltzmann constant, T_0 is the ambient temperature.

To study the diffusion behavior of the coupled Brownian motor, the variance of the position of the center of mass of the coupled Brownian particle $x_c(x_c = \frac{x_1+x_2}{2})$ can be used to calculate the effective diffusion coefficient of the system *Deff*:

$$Deff = \lim_{t\to\infty} \frac{1}{2}\frac{d}{dt}\langle [x_c - \langle x_c(t) \rangle]^2 \rangle, \quad (6)$$

In the formula, <…> denotes ensemble average, and $\langle [x_c(t) - \langle x_c(t)\rangle]^2\rangle = \langle x_c^2(t)\rangle - \langle x_c(t)\rangle^2$. Therefore, the effective diffusion coefficient of the coupled Brownian particle D*eff* is further expressed in the following form:

$$Deff = \lim_{t\to\infty} \frac{1}{2}\frac{d}{dt}\left(\langle x_c^2(t)\rangle - \langle x_c(t)\rangle^2\right). \quad (7)$$

In this paper, the Langevin equation is solved numerically by Runge-Kutta algorithm, and the effective diffusion coefficient of coupled Brownian particles *Deff* can be further obtained by combining with equation (7).

3. Runge-kutta algorithm of coupled Brownian ratchet

First, the Runge-Kutta algorithm can be applied to calculate the position of the 1 particle and the position of the 2 particle x_1 and x_2. Among them, the numerical solution procedure for particle 1 is as follows:

$$x_1(t+h) = x_1(t) + \frac{1}{2}h(F_{11} + F_{12}) + \sqrt{2Dh}Y_1, \quad (8)$$

$$F_{11} = \frac{\partial U(x_1(t))}{\partial x_1}, \quad (9)$$

$$F_{12} = \frac{\partial U(x_1(t) + hF_{11} + \sqrt{2Dh}Y_1)}{\partial x_1}, \quad (10)$$

2 Particle positions are calculated as follows

$$x_2(t+h) = x_2(t) + \frac{1}{2}h(F_{21} + F_{22}) + \sqrt{2Dh}Y_2, \quad (11)$$

$$F_{21} = \frac{\partial U(x_2(t))}{\partial x_2}, \quad (12)$$

$$F_{22} = \frac{\partial U(x_2(t) + hF_{21} + \sqrt{2Dh}Y_2)}{\partial x_2}. \quad (13)$$

Where Y_1 and Y_2 are Gaussian random numbers with a mean of zero and a variance of 1, h is the step length of the numerical calculation.

The position of the center of mass of the coupled Brownian particle can be calculated by the results of equations (9) and (12), and the further effective diffusion coefficient *Deff* can be obtained by equation (8). For the convenience of calculation, it can be simplified to the following form:

$$Deff = \frac{\langle x_c^2(t)\rangle - \langle x_c(t)\rangle^2}{2t}. \quad (14)$$

For the diffusion process, the asymptotic time evolution of the variance is usually a function of increasing time, satisfying the following power law.

$$\langle \Delta x_i^2(t)\rangle \sim t^{\alpha}. \quad (15)$$

The exponent α in the above formula can reflect the diffusion type of the system. At that time, α = 1 was

normal diffusion. At $0 < \alpha < 1$ time, the system behaved as underdiffusion, and at $\alpha > 1$ time, it was superdiffusion. It is easy to know that in the case of underdiffusion, the position variance increases more slowly with time than normal diffusion, while overdiffusion is faster than normal diffusion. Therefore, the time-dependent diffusion coefficient *Deff* can distinguish between these anomalous intermediate diffusion regions, that is, when *Deff* increases with time, it indicates superdiffusion, when *Deff* decreases with time, it corresponds to subdiffusion, and when *Deff* constant, the system behaves as normal diffusion. It is worth noting that only then is $\alpha \rightarrow 1$ the time-independent diffusion coefficient *Deff* given by equation (6).

4. Conclusion

In this paper, the diffusion of coupled Brownian particles is studied theoretically by the Langevin equation, the motion equation is solved numerically by the Runge-Kutta algorithm, the centroid position of coupled Brownian particles is obtained, and the effective diffusion coefficient *Deff* of coupled ratchets is further obtained. The diffusion research of coupled Brownian particles has shown significant theoretical value and practical significance in many fields. Through numerical simulation methods, researchers can deeply explore the dynamics of complex systems and provide references for theoretical exploration and experimental research in related fields. Especially in the field of biophysics, the model is often used to explain the motion mechanisms of various biological macromolecules, such as the energy conversion process of molecular motors, the spatial conformation change of proteins, and the migration behavior of receptors on the surface of cell membranes. Importantly, by numerically solving the effective diffusion coefficients, researchers can more accurately understand the movement of these biomolecules in the complex intracellular environment and thereby elucidate the underlying mechanisms of their biological functions. In the field of soft condensed matter physics, the model provides a powerful tool for the study of the microdynamics of colloidal dispersion systems and polymer solutions. In particular, the quantitative analysis of the effective diffusion coefficient plays an important role in exploring the mechanism of the interaction between particles affecting the macroscopic properties of the system. For example, the quantitative analysis provides a theoretical reference for understanding the rheological properties and phase behavior changes of materials. In addition, in the field of environmental science, the model can also be used to describe the migration and diffusion process of pollutant particles in complex media, providing a theoretical basis for environmental governance.

Disclosure statement

The authors declare no conflict of interest.

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