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Research on Directional Transport of Coupled Brownian Ratchet

Yuhang Lai, Xinran Ma, Meiqi Li, Liming Fan*

College of Physical Science and Technology, Shenyang Normal University, Shenyang 110034, Liaoning, China

***Corresponding author:** Liming Fan, lmfan@synu.edu.cn

Abstract: Molecular motors, as important nanomachines in cells, drive directional motion through ATP hydrolysis and play a key role in life processes such as DNA replication and material transport. In this paper, the kinetic evolution of coupled Brownian particles is described based on the overdamped Langevin equation, and the mean velocity of the coupled particles is obtained. By using the second-order Runge-Kutta algorithm, the dynamic characteristics of the directional transport of the coupled ratchet system can be studied theoretically. This research can provide a new approach for the design of nanomechanics and the mechanism analysis of biomolecular motion.

Keywords: Coupled Brownian ratchet; Langevin equation; Mean velocity of center of mass; Runge-Kutta algorithm

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1. Introduction

Brownian motors, also known as Brownian ratchets, are systems that can convert unbalanced drives into directional motion of Brownian motors in asymmetrical periodic potentials (ratchets). The system can be modeled as a coupled Brownian particle, and exploring the statistical properties of its directional transport is an important scientific problem [1–4]. In particular, the statistical parameters of the Brownian motor, such as speed, efficiency, diffusion coefficient, and Pe number, have received wide attention [5–8].

Biomolecular motors exist in the interior of cells and are proteases that achieve mutual conversion between chemical reactions and directional movements. Their dimensions are several or tens of nanometers, making them a kind of natural nanomachines. Molecular motor can catalyze the hydrolysis of ATP and use its released energy, because the motor itself is designed very delicate structure, the chemical energy released by the local process can further promote the motor to produce a larger size conformational change, as long as the motor and the orbital combination, this idea change will make it produce the corresponding relative motion, thus having the "movement." Studies have shown that molecular motors play an important role in all the basic processes of life, such as DNA replication, gene transcription, translation, material transport, ATP synthesis, and muscle contraction. As a result,

diseases related to molecular motors have been discovered. For example, myosin mutations are associated with dilated or hypertrophic cardiomyopathy; Cardiovascular diseases, for example, are associated with overexpression of a certain driver gene.

Various models of the Brown ratchet are derived from Feynman's ratchet and pawl system, which consists of a so-called ratchet and a pawl [9]. The ratchet is reminiscent of a circular saw with asymmetrical, serrated teeth, and the pawl allows the teeth to move effortlessly in one direction, eliminating rotation in the opposite direction. The ratchet and pawl are connected by a shaft with a windmill, the blades of which are surrounded by gas at a temperature of T1. The ratchet and pawl are kept at different temperatures of T2 (T2<T1). Random collisions of surrounding gas molecules with the blades will cause the ratchet to spin forward. This thermal noise correction can be used to perform tasks such as lifting loads.

In earlier studies of the ratchet model, the structure of the motion protein was completely ignored, treating it as a point Brownian particle with no internal degrees of freedom. The individual Brownian particles were small in speed and efficiency compared to the experimental data. In fact, the motor protein is usually a dimer. A conventional motor protein consists of two identical proteins connected by a neck region, each with a motor domain (head) and a carrier-binding domain. Recently, some authors have studied the transport of two coupled particles theoretically. For example, Klumpp et al. considered the multiplicative potential fluctuation problem in the case of strong coupling [10]; Stratopoulos et al. have proposed a simple Newtonian model where two motor head particles are connected by a neck coil spring [11]; Dan and Jayannavar consider the inverse correlation coupling case [12]. Wang and Bao studied the transport of two coupled particles in a ratchet potential [13].

In this paper, the coupled Brownian particles in a ratchet of arbitrary coupling strength are studied, and the transport characteristics of the coupled Brownian (motor) are discussed by a numerical method [14–15]. This study will help to understand the rich behavior of molecular motion in cells.

2. Theoretical study of coupled Brownian ratchet

In the microscopic environment inside the cell, the movement of the molecular motor is limited by many factors. This paper mainly studies the motion of coupled Brownian motors under asymmetric periodic potential, whose dynamic behavior can be described by the dimensionless overdamped Langevin equation:

$$\dot{x}_i = -\frac{\partial W_i}{\partial x_i} + \xi_i(t), \quad i = 1,2, \tag{1}$$

Where the x_i coordinates represent the *I*-th Brownian particle, W_i represents the potential energy of the *I*-th particle, and its expression is:

$$W_i = U_i + V_i, \tag{2}$$

In the above equation, U_i represents the interaction potential between two elastic coupled particles:

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

k is the coupling strength between particles, a is the coupling free length. V_i is the external force to which the

I-th Brownian particle is subjected:

$$V_i(x_i) = -V_0\left[\sin(\frac{2\pi\pi_i}{l}) + \frac{\Delta}{4}\sin(\frac{4\pi\pi_i}{l})\right], \quad (4)$$

Where V_0 is the barrier height of the external potential, Δ is the degree of asymmetry, *l is* the period of the external potential. In the formula (1), ξi(t) is Gaussian white noise, which satisfies the following statistical relationship.

$$\langle \xi_i(t) \rangle = 0, \quad (5)$$

$$\langle \xi_i(t) - \xi_j(t') \rangle = 2D_0\delta_{ij}\delta(t - t'), \quad (6)$$

In the formula, *i,j=1,2*, $D_0 = \gamma k_B T$, is thermal noise intensity, and γ is the damping coefficient; k_B is the Boltzmann constant, and T is the temperature environment.

To further study the directional transport of the Brownian ratchet, this paper uses the mean velocity of the centroid of the Brownian ratchet to calculate the speed of the quantized directional transport. The mean velocity of the centroid of the *I*-th Brownian particle is

$$\langle v_i \rangle = \mathrm{m}_{n\tau\to\infty}\ \frac{1}{n\tau}\int_{t_0}^{n\tau+t_0} \dot{x}_i(t)dt, i = 1,2, \quad (7)$$

In the formula, τ is the period time, *n* is the number of periods of system evolution, t0 is the initial moment, nτ represents the evolution time of coupled particles, and < > represents the ensemble average.

3. Algorithm implementation of coupled Brownian ratchet

The numerical simulation method of the Langevin equation has been widely used in the study of Brownian ratchet transport, and the second-order Runge-Kutta method is mainly used in this study.

First of all, set the initial value y = y(x) ∈ [a, b], according to the differential mean value theorem, there must be $\zeta \in [x_n, x_{n+1}]$, so

$$y(x_{n+1}) = y(x_n) + h\dot{y}(\zeta) = y(x_n) + hf(\zeta, y(\zeta)) \quad (8)$$

Set $y_n = y(X_n)$ and remember K* = F(ξ ,y(ξ)), then

$$y(x_{n+1}) = y_n + hK^* \quad (9)$$

In the formula, K^* is y(x) the average slope on $[x_n, x_{n+1}]$ top. So, by giving the average slope K^* an algorithm, the equation (9) can be turned into a numerical formula, for example, K^* by substituting $K_1 = f(x_n + y_n)$, that is Euler's formula, and then continuing to $K_2 = f(x_{n+1} + y_{n+1})$ substitute K^*, one can get the backward Euler formula, and then K_1, K_2 substitute the average value of K^*, one can get the two echelon formula. Suppose that if one can predict the slope of $[x_n, x_{n+1}]$ more points, and also use their weighted average instead, one can get a numerical

solution with higher precision K^*, which is the basic idea of the Runge-Kutta algorithm.

Runge-kutta formula in general form:

$$\begin{cases} y_{n+1} = y_n + h\sum_{i=1}^{r} c_i k_i \\ K_1 = f(x_n, y_n) \\ K_i = f\left(x_n + \lambda_i h, y_n + h\sum_{j=1}^{i-1} \mu_{ij} K_j\right) \end{cases} \tag{10}$$

Where K_i is the predicted value of y = y(x), the slope at the $x_n + \lambda_i h(0 \le \lambda_i \le 1)$ point; c_i,λ_i,μ_{ij}, are constants chosen to improve the accuracy of formula (10).

According to the general form of the Runge-Kutta algorithm (which is taken from the formula i = 1,2 and i is a positive integer), the numerical algorithm for the position of the first particle through the formula (8) and (9) is as follows.

$$x_1(t+h) = x_1(t) + \frac{1}{2}h(F_{11} + F_{21}) + \sqrt{2Dh}Y_1, \tag{11}$$

Where

$$F_{11} = f\big(x_1(t)\big), \tag{12}$$

$$F_{21} = f\big(x_1(t) + hF_{11} + \sqrt{2Dh}Y_1\big), \tag{13}$$

The position of the second particle is

$$x_2(t+h) = x_2(t) + \frac{1}{2}h(F_{12} + F_{22}) + \sqrt{2Dh}Y_2, \tag{14}$$

Among

$$F_{21} = f\big(x_2(t)\big), \tag{15}$$

$$F_{22} = f\big(x_2(t) + hF_{21} + \sqrt{2Dh}Y_2\big), \tag{16}$$

Where Y_2 is a standard Gaussian random number, that is, the mean is 0 and the variance is 1. Y_1 Formulas (11) and (14) are the numerical simulation calculations used in this paper. Accordingly, it can be calculated as follows.

$$\langle v_1 \rangle = \lim_{t\to\infty} \frac{\langle x_1(t)\rangle - \langle x_{01}(t)\rangle}{t}, \tag{17}$$

$$\langle v_2 \rangle = \lim_{t\to\infty} \frac{\langle x_2(t)\rangle - \langle x_{02}(t)\rangle}{t}, \tag{18}$$

Further, the mean velocity of the center of mass of the coupled particle:

$$\langle v \rangle = \frac{\langle v_1\rangle + \langle v_2\rangle}{2}, \tag{19}$$

Where, $x_1(t)$, $x_2(t)$ denotes the position of the coupled particle at time t; $x_{01}(t)$, $x_{02}(t)$ represents the position of the coupled particle at the initial moment. According to formula (19), the directional transport problem of a multi-

body coupled system can be studied numerically.

4. Conclusion and prospect

In recent years, Brown motor's directional transport has attracted extensive attention from scholars, and a lot of results have been achieved. Brownian motors are capable of transforming unbalanced drive into directional motion, a property that makes them of vital significance in many subject fields, such as biology and physics. Molecular motors inside cells, in particular, function as natural nanomachines and are involved in almost all the fundamental processes of life, such as DNA replication, gene transcription, and material transport. These molecular motors are only a few or tens of nanometers in size, but they can efficiently catalyze the hydrolysis of ATP, use the released chemical energy to promote their own conformational changes, and then produce directional motion. In this study, the coupled Brownian ratchet model is used to build a theoretical model of the molecular motor, and the directional transport speed of the molecular motor is further discussed by the numerical algorithm.

In this paper, the dimensionless overdamped Langevin equation is used to describe the directional motion of the coupled Brownian motor under asymmetric periodic potential. At the same time, the mean velocity of the center of mass is introduced to describe the speed of directional transport. In the aspect of numerical simulation, this paper gives the concrete process of solving the motion equation by the second-order Runge-Kutta algorithm. Based on the differential mean value theorem, the algorithm improves the precision of the numerical solution by predicting the slope of multiple points and taking the weighted average. Compared with the traditional Euler method, the Runge-Kutta algorithm shows higher accuracy and stability when dealing with the Langevin equation of coupled particles and can simulate the dynamic behavior of particles in a complex coupled environment more accurately, which greatly saves the time cost. However, the Runge-Kutta algorithm has certain requirements for the continuity of the solution, and its accuracy may not be as good as that of Euler's method when dealing with problems with poor continuity. Therefore, in the practical application, it is necessary to choose the appropriate algorithm according to the characteristics of the specific problem to ensure the accuracy and reliability of the simulation results.

The theoretical research method in this paper can be applied to the design of nanomachines and particle separation technology. In the following work, the researchers can further optimize the algorithm, develop the self-adaptive step length Runge-Kutta algorithm, combine machine learning and artificial intelligence technology to optimize the parameter selection, and improve the performance and adaptability of the algorithm in complex scenarios; In addition, further expand on theoretical issues, expand the connection between Langevin equation of coupled particles and theories ~~such as~~ quantum mechanics, study the collective behavior and directional motion of multi-particle coupled systems under quantum effects, build a solid theoretical foundation for understanding the macro properties of complex systems, and promote the development and innovation in related fields.

Disclosure statement

The authors declare no conflict of interest.

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