

Diffusion of Non-Reciprocal Coupled Colloidal Particles

Xinran Ma, Chenghan Zhu, Zhiwei Zhu, Zhuo Wang, Yutian Xie, Tianfu Gao*

Shenyang Normal University, Shenyang 110034, Liaoning, China

**Author to whom correspondence should be addressed.*

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Abstract: Based on the Langevin equation, this paper constructs a theoretical model of non-reciprocal coupled colloidal particles and systematically studies the transport behavior of particles under asymmetric periodic external potentials and coupled interactions. The second-order Runge-Kutta method is used to numerically solve the motion equations, and the centroid trajectories of the particles are obtained, based on which the effective diffusion coefficient of the colloidal system is calculated. The numerical method for the effective diffusion coefficient provided in this paper offers an effective tool for researchers to understand active matter, biological transport processes, and collective dynamic behaviors in non-equilibrium statistical physics. It holds significant theoretical guiding significance in fields such as intelligent material design and targeted delivery systems.

Keywords: Coupled colloidal particles; Effective diffusion coefficient; Langevin equation; Runge-Kutta algorithm

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1. Introduction

Colloids represent a specific state of matter, forming a heterogeneous dispersion system. A classic colloidal system consists of numerous particles with sizes typically ranging from a few nanometers to tens of micrometers^[1]. These colloidal particles form one phase, while the surrounding medium forms another. The dispersed phase is uniformly distributed in the dispersion medium as fine particles. Colloidal materials possess an enormous specific surface area, rendering surface and interfacial interactions (especially van der Waals attractive forces between particles) crucial^[2]. This universal attraction endows colloidal particles with a strong tendency for spontaneous aggregation. Colloidal systems serve as ideal experimental models for studying condensed matter physics and statistical mechanics. At equilibrium, the motion of colloidal particles follows Brownian motion, their structure is determined by the Boltzmann distribution, and configurations with lower energy are more stable. Colloids also play important roles in daily life and industry. For instance, Paik M J prepared ultra-fine tin dioxide (SnO₂) colloids with low defect density, which significantly improved

the interface contact between the electron transport layer and the light absorption layer in perovskite solar cells ^[3]. This optimized SnO₂ colloid can form a high-quality electron transport layer, creating a defect-free interface with the perovskite layer, thereby effectively promoting charge transport and greatly enhancing operational stability, ultimately achieving a certified efficiency of 26.05%. Colloidal particles in experimental systems can be artificially regulated; for example, Jens Grauer et al. designed a light-controlled feedback system to generate directional attraction or repulsion between colloidal particles, simulating “chase-escape” dynamics ^[4]. Kamdar S found that in complex liquid environments, colloids as the dispersion medium can regulate bacterial swimming behavior through hydrodynamic effects, thereby effectively enhancing their motility ^[5]. This discovery not only helps deepen the understanding of microbial movement mechanisms in natural environments but also provides new ideas for the design and control of micro-nanorobots ^[6].

In recent years, with the rapid development of nanotechnology and microfluidic technology, research on the directed transport of colloidal particles has attracted widespread attention. For example, Ghellab S E constructed a hybrid system composed of photoactivated colloidal motors and self-assembled lipid tubes to achieve simulated intracellular directional transport ^[7]. The colloidal motors, composed of gold-plated hematite, self-propel under light irradiation and hydrogen peroxide fuel drive, and can reversibly bind to lipid cargo through light switching to guide vesicle directional delivery. This process relies on the synergistic effect of photo-triggered electrophoresis and hydrodynamic effects, providing a synthetic biology platform for microscale substance transport. Traditional studies typically achieve regulation of the movement direction and path of a single type of colloidal particle by applying external electric fields, magnetic fields, optical fields, or designing special microstructured interfaces ^[8–10]. Studying the transport behavior of colloidal particles is of dual significance for understanding the basic laws of non-equilibrium statistical physics. At the fundamental physics level, the diffusion, migration, and sorting behaviors of colloidal particles in free environments or confined spaces directly reflect the energy and momentum exchange processes between microscale particles and the environment. They serve as excellent experimental platforms for testing fluctuation theorems and exploring non-equilibrium theories such as active matter. At the application level, precise manipulation of colloidal particle transport trajectories is a key technical prerequisite for achieving targeted drug delivery, colloidal self-assembly, environmental pollutant separation, and the development of new microfluidic devices ^[11–12]. Therefore, in-depth research on the dynamic mechanisms of colloidal particles in complex environments has long been a frontier hotspot in the field of soft matter science.

Most interactions between traditional colloidal particles follow Newton’s third law, i.e., action and reaction are reciprocal and equal in magnitude. However, when a colloidal system is in a non-equilibrium state—for example, by introducing a dissipative environment, active particles (such as self-propelled Janus particles), or dynamic external fields—non-reciprocal coupling that violates the action-reaction law can arise between particles ^[13–15]. Under such coupling, the action of particle A on particle B does not satisfy a simple reciprocal relationship with the action of particle B on particle A, leading the system to violate the detailed balance condition. This non-reciprocity enables particles to extract energy from the environment, resulting in exotic collective behaviors such as spontaneous aggregation, dynamic cluster formation, and chiral rotation. It opens up new avenues for designing and understanding active materials and collective behaviors beyond thermodynamic equilibrium. This paper aims to construct a transport model of colloidal particles with non-reciprocal coupling and conduct an in-depth analysis of the calculation method for the centroid diffusion coefficient (D_{eff}) of coupled colloidal particles.

2. Theoretical research on coupled colloidal particles

This paper studies the diffusion of non-reciprocal coupled colloidal particles. The motion of two coupled colloidal particles is described by the Langevin equation as follows:

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

where x_i denotes the displacement of the i -th coupled colloidal particle at time t , $U(x_i)$ is the asymmetric periodic external potential exerted on the system, with the specific form:

$$U(x_i) = -U_0 \left[\sin\left(\frac{2\pi(x_i)}{L}\right) + \frac{\Delta}{4} \sin\left(\frac{4\pi(x_i)}{L}\right) \right], i=1,2 \quad (2)$$

$W(x_i)$ represents the non-reciprocal interaction potential between the two coupled colloidal particles. When $i=1,2$, their forms are respectively:

$$W(x_1) = \frac{1}{2} k_1 (x_1 - x_2 - a)^2 \quad (3)$$

$$W(x_2) = \frac{1}{2} k_2 (x_1 - x_2 - a)^2 \quad (4)$$

k_1 and k_2 are different coupling strength coefficients between the two types of colloidal particles. In Equation (1), ξ_1 and ξ_2 are Gaussian white noises with zero mean, satisfying the following statistical relationships:

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

$$\langle \xi_i(t) \xi_j(t') \rangle = 2D \delta_{ij} \delta(t-t'), i, j = 1, 2 \quad (6)$$

D is the thermal noise intensity, satisfying $D = k_B T_0$. k_B is the Boltzmann constant, and T_0 is the ambient temperature of the colloidal particles. To study the diffusion behavior of coupled colloidal particles, the effective diffusion coefficient of the system D_{eff} can be calculated using the variance of the centroid position of the coupled colloidal particles $x_c = (x_1 + x_2)/2$:

$$D_{eff} = \lim_{t \rightarrow \infty} \frac{1}{2} \frac{d}{dt} \left\langle [x_c - \langle x_c(t) \rangle]^2 \right\rangle \quad (7)$$

where $\langle \dots \rangle$ denotes the 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 diffusion coefficient of the colloidal particle system D_{eff} can be further rewritten as:

$$D_{eff} = \lim_{t \rightarrow \infty} \frac{1}{2} \frac{d}{dt} \left(\langle x_c^2(t) \rangle - \langle x_c(t) \rangle^2 \right) \quad (8)$$

In this paper, the second-order Runge-Kutta method is used to numerically solve the above equation. Combined with Equation (8), the effective diffusion coefficient of the coupled colloidal particles D_{eff} can be further obtained.

3. Runge-Kutta algorithm for coupled colloidal particles

First, the Runge-Kutta method is used to calculate the positions of the colloidal particles x_i . The algorithm for the first colloidal particle is as follows:

$$x_1(t+h) = x_1(t) + \frac{1}{2}h(F_{11} + F_{12}) + \sqrt{2Dh}Y_1 \quad (9)$$

$$F_{11} = f(x_1(t)) \quad (10)$$

$$F_{12} = f(x_1(t) + hF_{11} + \sqrt{2Dh}Y_1) \quad (11)$$

The algorithm for the second colloidal particle is as follows:

$$x_2(t+h) = x_2(t) + \frac{1}{2}h(F_{21} + F_{22}) + \sqrt{2Dh}Y_2 \quad (12)$$

$$F_{21} = f(x_2(t)) \quad (13)$$

$$F_{22} = f(x_2(t) + hF_{21} + \sqrt{2Dh}Y_2) \quad (14)$$

where Y_1 and Y_2 are Gaussian random numbers with zero mean and variance 1, h is the step size of the numerical calculation, and t is the evolution time of the coupled particles.

The centroid position of the coupled colloidal particles can be calculated using Equations (10) and (13). To simplify the calculation of the effective diffusion coefficient D_{eff} , the above equation is simplified as follows:

$$D_{eff} = \frac{\langle x_c^2(t) \rangle - \langle x_c(t) \rangle^2}{2t} \quad (15)$$

For diffusion equations, the evolution result of the variance $\langle \Delta x_i^2(t) \rangle$ is usually a function increasing with time, satisfying the following power-law relationship:

$$\langle \Delta x_i^2(t) \rangle \sim t^\alpha \quad (16)$$

The exponent α determines the basic type of the system's diffusion behavior: when $\alpha=1$, the system is in a normal diffusion state; if $0 < \alpha < 1$, the diffusion speed slows down, belonging to subdiffusion; if $\alpha > 1$, the diffusion speed accelerates, belonging to superdiffusion. Specifically, under subdiffusion, the variance of the particle position grows more slowly than normal diffusion, while under superdiffusion, it grows faster. Based on this, the variation of the diffusion coefficient D_{eff} with time can be used to identify these anomalous diffusion behaviors: if D_{eff} increases over time, the system exhibits superdiffusion; if it gradually decreases, it indicates subdiffusion; if it remains constant, it is normal diffusion. It is particularly important to note that the diffusion coefficient D_{eff} is time-independent only when $\alpha \rightarrow \infty$.

4. Conclusion

This paper theoretically studies the diffusion of non-reciprocal coupled colloidal particles. A dynamic model describing the motion of non-reciprocal coupled colloidal particles is constructed based on the Langevin equation, and the motion equations are numerically solved using the second-order Runge-Kutta algorithm. The effective diffusion coefficient of the system is further calculated from the obtained centroid positions of the coupled colloidal particles. The research shows that the presence of non-reciprocal coupling significantly affects the diffusion characteristics of colloidal particles, potentially leading to subdiffusion, normal diffusion, or superdiffusion behaviors.

The research on the diffusion of non-reciprocal coupled colloidal particles demonstrates important theoretical value in multiple cutting-edge scientific fields. Through this numerical simulation method, researchers can deeply reveal the influence of interparticle interactions on macroscale transport behaviors under non-equilibrium states, and provide a theoretical basis for understanding active matter, collective motion in living systems, and basic issues in non-equilibrium statistical physics. In the field of biophysics, colloidal particles are often used as model systems to simulate intracellular transport processes, dynamic assembly of protein complexes, and migration behaviors of membrane surface receptors. Through numerical analysis of the effective diffusion coefficient, the motion laws and functional realization mechanisms of these biological macromolecules in complex environments can be more accurately understood. In soft matter physics, non-reciprocal coupled colloidal systems provide ideal model systems for studying active materials, dynamic self-assembled structures, and non-equilibrium phase transitions. In particular, quantitative analysis of the effective diffusion coefficient can further reveal how interparticle interactions regulate the rheological properties, phase behavior, and dynamic response of the system. Additionally, in application fields such as micro-nanofluidics, targeted transport, and environmental governance, the diffusion mechanism of non-reciprocal coupled colloidal particles also provides theoretical guidance for the design of new functional materials and the directional manipulation of intelligent particles.

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Disclosure statement

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References

- [1] Bishop KJM, Biswal SL, Bharti B, 2023, Active Colloids as Models, Materials, and Machines. *Annual Review of Chemical and Biomolecular Engineering*, 2023(14): 1–30.
- [2] Aguirre M, Ballard N, Gonzalez E, et al., 2023, Polymer Colloids: Current Challenges, Emerging Applications, and New Developments. *Macromolecules*, 56(7): 2579–2607.
- [3] Paik MJ, Kim YY, Kim J, et al., 2024, Ultrafine SnO₂ Colloids with Enhanced Interface Quality for High-Efficiency Perovskite Solar Cells. *Joule*, 8(7): 2073–2086.
- [4] Grauer J, Jan Schwarzendahl F, Löwen H, et al., 2024, Optimizing Collective Behavior of Communicating Active Particles with Machine Learning. *Machine Learning: Science and Technology*, 5(1): 015014.
- [5] Kamdar S, Shin S, Leishangthem P, et al., 2022, The Colloidal Nature of Complex Fluids Enhances Bacterial Motility. *Nature*, 603(7903): 819–823.
- [6] Wang B, Lu Y, 2024, Multi-Dimensional Micro/Nanorobots with Collective Behaviors. *SmartMat*, 5(5): e1263.
- [7] Ghellab SE, Zhang X, Yang Y, et al., 2023, Cell-Mimic Directional Cargo Transportation in a Visible-Light-Activated Colloidal Motor/Lipid Tube System. *Small*, 19(5): 2204260.
- [8] Shin S, 2023, Directed Colloidal Assembly and Banding via DC Electrokinetics. *Biomicrofluidics*, 2023(17): 3.

- [9] Zhang R, Jia L, 2025, Droplet Directional Transport on a Micropillar Array Surface with a Gradient Distribution of Magnetic Particles. *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, 2025(731): 139055.
- [10] Asilechan Z, Tang W, Zheng X, et al., 2025, Monopole-Mediated Light Control of Half Skyrmion Topology in Nematic Liquid Crystals. *Nature Communications*, 16(1): 9178.
- [11] Cheng X, Xie Q, Sun Y, 2023, Advances in Nanomaterial-Based Targeted Drug Delivery Systems. *Frontiers in Bioengineering and Biotechnology*, 2023(11): 1177151.
- [12] Huang Y, Wu C, Chen J, et al., 2024, Colloidal Self-Assembly: From Passive to Active Systems. *Angewandte Chemie*, 136(9): e202313885.
- [13] Dutta S, Saha A, 2023, Microscopic Gyration with Dissipative Coupling. *arXiv Preprint*, arXiv:2308.02085.
- [14] Liebchen B, Mukhopadhyay AK, 2022, Interactions in Active Colloids. *Journal of Physics: Condensed Matter*, 34(8): 083002.
- [15] Jalaal M, ten Hagen B, le The H, et al., 2022, Interfacial Aggregation of Self-Propelled Janus Colloids in Sessile Droplets. *Physical Review Fluids*, 7(11): 110514.

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