Physica A 436 (2015) 126–134

Contents lists available at ScienceDirect

Physica A

journal homepage: www.elsevier.com/locate/physa

Stochastic dynamics of coupled active particles in an overdamped limit

Minjung Ann [a], Kong-Ju-Bock Lee [a,*], Pyeong Jun Park [b,*]

[a] Department of Physics, Ewha Womans University, Seoul 120-750, Republic of Korea

[b] School of Liberal Arts and Sciences, Korea National University of Transportation, Chungju, 380-702, Republic of Korea

HIGHLIGHTS

- A new coupled active Brownian dynamics model in an overdamped limit is proposed.
- The active force includes two parameters determining direction and strength.
- For an application, a cargo transport by molecular motors in a cell is adopted.
- The results are consistent with well-known observation for the cargo transport.

ARTICLE INFO

Article history:
Received 30 October 2014
Received in revised form 28 March 2015
Available online 11 May 2015

Keywords:
Stochastic dynamics
Active particle
Overdamped limit
Cellular transport

ABSTRACT

We introduce a model for Brownian dynamics of coupled active particles in an overdamped limit. Our system consists of several identical active particles and one passive particle. Each active particle is elastically coupled to the passive particle and there is no direct coupling among the active particles. We investigate the dynamics of the system with respect to the number of active particles, viscous friction, and coupling between the active and passive particles. For this purpose, we consider an intracellular transport process as an application of our model and perform a Brownian dynamics simulation using realistic parameters for processive molecular motors such as kinesin-1. We determine an adequate energy conversion function for molecular motors and study the dynamics of intracellular transport by multiple motors. The results show that the average velocity of the coupled system is not affected by the number of active motors and that the stall force increases linearly as the number of motors increases. Our results are consistent with well-known experimental observations. We also examine the effects of coupling between the motors and the cargo, as well as of the spatial distribution of the motors around the cargo. Our model might provide a physical explanation of the cooperation among active motors in the cellular transport processes.

1. Introduction

Schweitzer et al. [1] proposed a model for active Brownian particles, and in their model, the active particles are able to absorb energy from the environment, store it in an internal energy depot, and then convert the stored energy into mechanical work. They considered a function proportional to the square of a particle's velocity as an energy conversion rate and discussed various dynamic properties of interesting active systems [2–5]. The model was generalized by considering

* Corresponding authors.
E-mail addresses: kjblee@ewha.ac.kr (K.-J.-B. Lee), pjpark@ut.ac.kr (P.J. Park).

http://dx.doi.org/10.1016/j.physa.2015.05.006
0378-4371/

the energy conversion rate to be a function of the particle's position and velocity [6], yielding the diverse patterns of motion of the active particle, including its braking mechanisms, spontaneous oscillations characterizing a negative stiffness, and stepping motions.

In order to model the active dynamics in the overdamped limit where the velocity is not a well-defined stochastic variable, we considered the energy conversion rate to be a function of the drift velocity, up to the quadratic order [7]. Since an active Brownian particle model in an overdamped limit is a plausible candidate to describe the dynamics of a processive molecular motor in a cell, kinesin-1 was analyzed using our model. Kinesin-1 is a well-known processive cytoskeletal motor that exhibits discrete unidirectional motion, and our model successfully captured the primary features of the motor, including its forward and backward steppings and the stalling against an external load force [7,8].

In this paper, we would like to investigate the dynamics of coupled active particles in the overdamped limit. The realistic system is composed of multiple motors that transport a cargo in a cell. The molecular motors play a crucial role in transporting the cargo particles, such as the vesicles and organelles in a cell. In many cases, several molecular motors are bound as a team to a common cargo and cooperatively move it. For most types of motors, the driving force on the cargo, as well as the run length of the motor–cargo complex, increases when the number of participating motors increases [9–11]. Interestingly, however, *in vivo* observations revealed that the number of processive cytoskeletal motors, kinesin-1, do not significantly affect the velocity and the run length of the cargo [12,13]. Various approaches were proposed to investigate cargo transport via processive or non-processive molecular motors and to experimentally and theoretically determine how the number of motors affects the intracellular transport mechanism [14–25].

We propose a model for the Brownian dynamics of coupled active particles that are harmonically bound to a passive particle, and perform Brownian dynamics simulation of the system by varying the number of coupled active particles, the coupling strength between the active and the passive particles, and the viscous friction. In this application, the active particles correspond to kinesin-1, and the passive particle corresponds to a cargo. In the simulation, some realistic parameters are adopted for kinesin-1, and we analyze the effects of the particle number, internal relaxation, and hydrodynamic drag on the dynamics of the system. For simplicity, our present model does not include the stochastic detachment of kinesin-1 from its track, even though it plays an important role in the cargo transport.

In Section 2, we construct a model for the dynamics of active particles bound to a passive particle based on our previous model [7]. The results of the active Brownian dynamics simulation follow in Section 3. Finally, summary and conclusion are given in Section 4.

2. Coupled active particle model

We briefly describe our previous model for the dynamics of a single active particle, and extend it to the case with many active particles that are coupled to a passive particle.

2.1. A single active particle

The overdamped stochastic equation for the motion of an active particle with its position $x(t)$ at time t is

$$\gamma \frac{\mathrm{d}x}{\mathrm{d}t} = F_{\text{ext}} + F_{\text{active}} + \xi(t), \tag{1}$$

where γ is the friction coefficient of the active particle, F_{ext} is the external force, and $\xi(t)$ is the Gaussian white noise. $\xi(t)$ is characterized by

$$\langle \xi(t) \rangle = 0 \tag{2}$$

$$\left\langle \xi(t)\xi(t') \right\rangle = 2\gamma k_B T \delta(t - t') \tag{3}$$

with T denoting the temperature and k_B the Boltzmann constant. The active force F_{active} is generated by converting the energy stored in an energy depot $e(t)$ at time t, and the time evolution of $e(t)$ is modeled as

$$\frac{\mathrm{d}e}{\mathrm{d}t} = q(t) - ce - F_{\text{active}} v_D, \tag{4}$$

where $q(t)$ is the rate of energy supply to the depot at time t, c is the spontaneous energy decay rate, and v_D is the drift velocity of the particle defined below.

We model the active force on the particle as

$$F_{\text{active}} = (a_1 + a_2 v_D)e, \tag{5}$$

where a_1 and a_2 are parameters determining direction and strength of the active force. v_D is the drift velocity of the particle, and it is defined by an instantaneous velocity in the absence of noise:

$$v_D = \frac{F_{\text{ext}} + a_1 e}{\gamma - a_2 e}. \tag{6}$$