Thermal fluctuation driven collective directed-motion due to coordinate-dependent damping

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In the present paper, we show thermal fluctuations driven directed transport of a collection of dimer in various configurations. The directed motion arises as a result of the existence of broken symmetry caused by coordinate or state dependence of the diffusivity and damping. In all the simulations, the diffusivity of particles are related to the damping coefficient in accordance with the Stokes-Einstein relation. We also show here that in the absence of the broken symmetry induced by the coordinate/state dependent diffusion, similar structures form, however they do not show directed transport on average. We also give in this paper a detailed discussion on the interpretation of such motions driven by bath degrees of freedom pertaining to conditions of equilibrium and out of equilibrium situations.

I. INTRODUCTION:

Flocking of birds, shoaling of fishes etc., are collective transports which generally are studied by the introduction of a non-equilibrium “self-driving” force in the context of active systems. One of the earliest models that displays flocking from an initially disordered configuration is the Vicsek model [1]. There are various variants of the Vicsek model present in literature [2–5]. Many models of active systems have been developed to demonstrate flocking transitions, pattern formation, swarming transitions [6–8], motility-induced phase separation (MIPS) [9–12]. Redner et al., has shown that an active colloidal system in thermal noise and excluded volume interaction displays phase separation into dense and dilute phases [10]. Martin et al., considered an assembly of active Brownian particles with excluded volume interaction and velocity aligning protocol shows emergence of flocking [7]. Liao et al., showed emergence of flocking in an assembly of active Brownian disks with steric-repulsion and dipole-dipole interactions [6].

In the present paper we show that thermal fluctuations alone can drive collective motion in the presence of coordinate or state dependent diffusion where no activation of the system is necessary. It has been shown by Bhattacharyay and coauthors [13–15] that a symmetry-broken dimer in the presence of coordinate dependent damping/diffusion, in general, can filter Brownian motion to produce directed transport. It has also been shown by Bhattacharyay and coworkers [16, 17] that in the presence of coordinate-dependent damping it is possible to keep Stokes-Einstein relation locally intact everywhere in a heat bath which ensures thermal equilibrium of the system.

Directed transport driven by thermal fluctuations can play its kinematic role in the collective functioning of objects undergoing structural transitions. The characteristic directed motion of structured objects driven by thermal-fluctuations can facilitate or hinder structural transitions on top of what the Kramers’-rate theory predicts. In biological systems such matching of structures is immensely important for functionality. In the stochastic dynamics of complex molecules and in various other systems coordinate- or state-dependence of diffusion is being identified to be a key ingredient [18–28]. Therefore, when the coordinate or state dependence of diffusion can result in directed transport of structured objects, its role in modifying our standard understanding of barrier overcoming transitions could potentially be immense.

We numerically explore various characteristic motion of a collection of interacting dimers. The collection of dimers interact by dipole-interactions where similar poles repel and opposite poles attract keeping intact the excluded volume. We have already shown that, in a one-dimensional space, a symmetry broken dimer will show directed motion caused by coordinate dependence of diffusion [13–15]. However, in a two (or higher) dimensional space, this directed motion of such an individual dimer will be lost due to the presence of rotational degrees of freedom. The tendency of such individual dimer to move directionally will manifest in driving collective motions in a many-body system where these dimers would from structures due to interactions with each other restricting rotational degrees of freedom of an individual. This is the motivation of the present numerical exploration that presents startling results akin to those of active systems in the absence of any non-equilibrium drive.

The next section of the paper gives an overview of the fundamentals underlying the passive directed motion of a symmetry-broken dimer. Following that we present the many-body model and specify all the conservative interactions present in the model. Then we present the scheme of the simulations followed by results in different parameter regimes. Finally, we present a discussion of the results and conclude.
II. FUNDAMENTALS OF PASSIVE DIRECTED MOTION OF A SYMMETRY-BROKEN DIMER

Consider over-damped equations of motion of a system of two particles at positions $x_1$ and $x_2$ as

$$\frac{dx_1}{dt} = -\frac{1}{\Gamma_1(z)} \partial V(z) \partial x_1 + \sqrt{\frac{2k_B T}{\Gamma_1(z)}} \eta_1(t),$$

$$\frac{dx_2}{dt} = -\frac{1}{\Gamma_2(z)} \partial V(z) \partial x_2 + \sqrt{\frac{2k_B T}{\Gamma_2(z)}} \eta_2(t).$$

(1)

where $z = x_1 - x_2$, $\eta_i(t)$ is Gaussian white noise of unit strength with no cross-correlation i.e. $\langle \eta_i(t) \eta_j(t) \rangle = \delta_{ij}$, $T$ is the temperature of the heat-bath and $k_B$ is the Boltzmann constant. Particles are characterized by having different damping coefficients $\Gamma_i(z)$ which depend on the configuration coordinate $z$ of the system. $V(z)$ generates a conservative force field between these particles which is attractive at a larger distance and is repulsive at small distances to account for an excluded volume interaction. Considering the centre of the dimer (or the system, since there is no mass) to be $x = \frac{x_1 + x_2}{2}$ one can rewrite the model as

$$\frac{dz}{dt} = -\left[ \frac{1}{\Gamma_1(z)} + \frac{1}{\Gamma_2(z)} \right] \partial V(z) \partial z + \xi_z(z,t),$$

$$\frac{dx}{dt} = -\frac{1}{\Gamma_1(z)} \partial V(z) \partial x + \xi_x(z,t).$$

(2)

where $\xi_z(z,t) = \sqrt{2k_B T} \left[ \frac{\eta_1(t)}{\sqrt{\Gamma_1(z)}} - \frac{\eta_2(t)}{\sqrt{\Gamma_2(z)}} \right]$ and $\xi_x(z,t) = \sqrt{k_B T} \left[ \frac{\eta_1(t)}{\sqrt{2\Gamma_1(z)}} + \frac{\eta_2(t)}{\sqrt{2\Gamma_2(z)}} \right]$. In (2), the configuration space has decoupled from that of the centre of the system. The average velocity of the centre of the system is

$$\langle \frac{dx}{dt} \rangle = -\left\langle \left[ \frac{1}{\Gamma_1(z)} - \frac{1}{\Gamma_2(z)} \right] \partial V(z) \partial z \right\rangle.$$

(3)

which in general is not zero for $\Gamma_1(z) \neq \Gamma_2(z)$ and $\left[ \frac{1}{\Gamma_1(z)} - \frac{1}{\Gamma_2(z)} \right]$ is the symmetry breaking term in the presence of coordinate dependence of damping, in general, and otherwise not when $\Gamma_i$’s are even different constants. [13–15].

It is important to note that even when $\langle \frac{dx}{dt} \rangle \neq 0$, the other average velocity $\langle \frac{dz}{dt} \rangle$ has to be identically zero under equilibrium conditions [13–15]. Equilibrium fluctuations of the system are function of the internal coordinate $z$ and there cannot be any average current existing on the centre of the dimer frame ($z$-coordinates) although the centre of dimer itself can maintain a constant average velocity.

There is no average motion of the centre of the dimer produced due to direct forcing of the system by the bath degrees of freedom because the bath is homogeneous and isotropic. However, this forcing intermittently brings the dimer to configurations which are of higher potential energy than the lowest potential energy configuration. The response of the dimer is to come back to the lowest potential energy configuration from the excited states. During this response, the damping of the constituents of the dimer being coordinate/state dependent, the two particles of the dimer move through different distances in unit time due to different damping despite being subjected to equal and opposite internal forces of interaction in each configuration. These response of the constituents of the dimer when are different during the attractive (confining) and repulsive (excluded volume) interactions, then only it creates an average displacement of the centre of the dimer. This is the reason even when $\Gamma_1 \neq \Gamma_2$, when $\Gamma_1$ and $\Gamma_2$ are constants, the system does not show any average motion of its centre and different $z$-dependence of the constituents of the dimer is the condition for the broken symmetry.

III. MANY DIMER MODEL

Let us consider $N$ such dimers interacting with each other in a thermal atmosphere at a constant temperature $T$. The similar constituents of different dimers i.e., those with the same $\Gamma_1(z)$ or $\Gamma_2(z)$ repel each other within some defined proximity and dissimilar constituents attract each other within certain distance keeping in place excluded volume interaction at small distances between them. These dimer are confined to a circular two-dimensional region. The equations of motion for $N$ such dimer are:

$$\frac{dr_i}{dt} = -\frac{1}{\Gamma_i} \nabla_{r_i} \left[ V_h(r_i, r_j) + V_b(r_i) \right] - \frac{1}{\Gamma_i} \nabla_{r_i} \left[ \sum_{j \neq i} \left[ V_l(|r_i - r_j|) + V_u(|r_i - r_j|) \right] \right] + \sqrt{\frac{2k_B T}{\Gamma_i}} \eta_i(t).$$

(4)
\[
\frac{dr_i^2}{dt} = \frac{1}{\Gamma_2} \nabla r_i^2 \left[ V_h(r_i^1, r_i^2) + V_b(r_i) \right] - \frac{1}{\Gamma_2} \nabla r_i^2 \left[ \sum_{j \neq i} \left[ V_j(|r_i^2 - r_j^2|) + V_u(|r_i^2 - r_j^2|) \right] \right] + \sqrt{\frac{2k_BT}{\Gamma_2}} \eta_i(t).
\]

Here, \( r_i^1 \) and \( r_i^2 \) are the positions of constituent 1 and constituent 2 of the \( i \)th dimer. The interaction potential between primary constituents of a dimer (constituent 1 and constituent 2) \( V_h \) is harmonic. \( \Gamma_1 \) and \( \Gamma_2 \) are the coordinate-dependent damping coefficients associated, respectively, to constituent 1 and constituent 2 of a dimer which remain similar for all dimers. \( \eta_1^i \) and \( \eta_2^i \) represent Gaussian white noise of zero mean and a unit strength. None of these noises are cross-correlated i.e. \( \langle \eta_k^i \eta_l^j \rangle = \delta_{ij} \delta_{kl} \). \( V_b \) is the confining potential due to circular boundary. \( V_l \) corresponds to repulsive interaction between the like (similar) constituents of different dimers.

\[
V_l(r_{ij}) = \begin{cases} \frac{1}{2} \kappa_l (r_{ij} - r_l)^2 & \text{if } r_{ij} < r_l, \\ 0 & \text{if } r_{ij} \geq r_l, \end{cases}
\]

where, \( r_{ij} \) is the magnitude of separation between same constituents of different dimers and \( \kappa_l \) is the repulsion strength. \( r_l \) is the distance below which the same constituents starts feeling repulsive force. The L-J potential and L-J force is defined as:

\[
V_{LJ}(r_{ij}) = 4\epsilon \left( \frac{\sigma_{ij}^6}{r_{ij}^6} - \frac{\sigma_{ij}^{12}}{r_{ij}^{12}} \right),
\]

\[
F_{LJ}(r_{ij}) = \frac{24\epsilon \sigma_{ij}^6}{r_{ij}^7} \left( \frac{2\sigma_{ij}^6}{r_{ij}^6} - 1 \right),
\]

\[
\phi_u(r_{ij}) = \frac{k_u}{2}(r_{ij} - r')^2,
\]

where, \( r_{ij} \) is the magnitude of separation between different constituents (monomers) of different dimers. \( k_u \) is the spring coefficient for repulsive interaction between unlike dimers of different monomers. \( V^*_{LJ} \) and \( F^*_{LJ} \) are the values of Lennard-Jones potential and force at cutoff distance \( r_c \) respectively. We set \( (r'/\sigma)^6 = 2, r_c = 4\sigma \) and \( \phi = \phi_u - \epsilon \), where \( \epsilon \) is the depth of well and \( \sigma \) is a length parameter.

**IV. SIMULATION SCHEME**

We transform 2N coupled Brownian equations originally in position coordinate to 4N coupled Brownian equations in cartesian system of coordinates for our simulation. We initialise dimers in random configuration and implement Euler-Maruyama algorithm to simulate these 4N coupled Brownian dynamics equations.

We use the following update scheme for our simulations:

1. Assign random positions to dimers at beginning of the simulation.
(2) Corresponding to the positions, calculate the respective forces.

(3) Update the position of each dimer using the forces calculated in step (2) by employing explicit Euler-Maruyama discretization scheme.

(4) Go back to step (2) and repeat.

Typical structures of the damping functions and the potentials are shown in Fig.1 and Fig.2 for a particular set of parameters.

![Fig. 1: Coordinate dependent damping associated with primary constituents (monomers) of symmetry broken dimers. [Left] figure shows the coordinate-dependent damping of monomer 1 with parameters: $a_1 = -0.3$, $b_1 = 0.4$, $r\text{min} = 1$ and $\lambda = 100$. [Right] shows the coordinate-dependent damping of monomer 2 with parameters: $a_2 = -0.1$, $b_2 = 0.3$, $r\text{min} = 1$ and $\lambda = 100$.](image)

![Fig. 2: Potentials: (a) Intra-dimer potential: $\alpha = 200$, $r\text{min} = 1$. (b) Confining potential: $k_T = 1000$, $R = 31$. (c) Like monomer interaction potential: $\kappa_{ij} = 80$, $r_{ij} = 2$. (d) Unlike monomer interaction potential: $k_2 = 60$, $\epsilon = 20$, $\sigma = 1$.](image)

V. RESULTS OF THE SIMULATIONS

The simulations are run for every set of parameters of interaction always under symmetry-broken and symmetry-unbroken conditions to compare the directed transport in the symmetry-broken case with the symmetry-unbroken case which does not show any average directed motion in the similarly formed many-body structures. Link of the movies of pair of such symmetry-broken and unbroken situations under exactly the same interaction parameters are given in the respective figure captions. A symmetry-broken case is, in general, there when $\Gamma(z) = 0.1$ i.e., equal to a constant. However, we have checked several symmetry-unbroken situations at a wide range of parameter values to observe no average directed motion. Similarly, the parameters of the functions of the symmetry-broken cases are for the best representation, however, we have checked the results over wider parameter ranges. The average velocity under symmetry-broken scenario would obviously depend on the value of the parameters in the damping function, but, there always are directed motions under the symmetry-broken conditions.

All simulations use a new random seed each time and it has been checked that qualitative results remain the same for given set of parameters independent of the random seed. We have set $k_BT$ and $r_{\text{min}}$ as our reference for energy and distance scale respectively and both have been set to unity. All parameters for symmetry-broken dimers have been fixed throughout the simulations and are the same as the ones mentioned in the captions of Fig.1 and Fig.2, except for $\sigma$ and $r_1$ which have been varied from case to case. $\Delta t$ denotes the discretised time element used in simulation. Videos have been produced by harnessing matplotlib library, using the data of positions of dimers for both symmetry broken case and a symmetry-unbroken case. In case the videos generated are long or too slow, they have then been sped up by using a video editor.

A. Characteristic motion of various structures

We ran the simulation for $5 \times 10^8$ iterations and recorded the positions of dimers every 100 iterations at parameter values given in the caption of Fig.3. Every step of iteration includes update of positions of all the particles by one time step. Starting from a random distribution of dimers, linear queued chains of dimers are formed. The chain-like flocks of dimers formed generally display linear transport unless they form a ring like structure that rotates in a particular direction. The direction of motion is indicated by arrows in all the figures.

In figure Fig.4, we show the results of simulation for $5 \times 10^7$ iterations where the positions of the dimers are recorded at every 1000 iterations in a different interaction regime. Initially small cyclic chains of associated tri-dimer and quad-dimer are formed. The intermediate structures formed by the association of the three and four dimers when exist in a closed loop form always rotate in a particular direction. The direction of the rotation is selected predominantly by the direction of motion of individual dimers. Many-body interactions in this parameter regime leads to aligned dimers akin to ferromagnetic order. This eventually forms a single cluster that swarms through on
FIG. 3: Parameters: $\sigma = 1.5, r_l = 3$ and $\Delta t = 10^{-4}$. In the sub-figures: (a) linearly and circularly arranged flocks shown at small times. (b) longer flocks develop at large times. The movie of the time evolution of these structures sped up by ten times can be found [here](#).

FIG. 4: Parameters: $\sigma = 2, r_l = 3$ and $\Delta t = 10^{-5}$. In the sub-figures: (a) Chiral symmetry broken objects and swarms shown at small times. (b) Swarm formed at long times, swarming around the inner periphery. The movie of the time evolution of these structures sped up by five times can be found [here](#).

FIG. 5: Parameters: $\sigma = 1, r_l = 1.8$ and $\Delta t = 10^{-5}$. In the sub-figures: (a) uni-directional rotating tri-dimers, quad-dimer and associated symmetry broken structures shown at small times. (b) An assembly of chiral symmetry broken rectangular lattice like structure shown at large times. The movie of the time evolution of these structures speeding up by ten times can be found [here](#).

FIG. 6: Parameters: $\sigma = 1, r_l = 2.2$ and $\Delta t = 10^{-4}$. In the sub-figures: (a) Associated dimer cluster and a ring of uni-directional rotating dimers. (b) Chiral symmetry broken triangular lattice like structure shown at large times. The movie of the time evolution of these structures speeding up by 1.5 times can be found [here](#).

In this paper we have explored the thermal directed motion of various structures formed by interacting dimers whose constituent particles have a configuration dependent damping and diffusion related by the Stokes-Einstein (fluctuation-dissipation) relation. This configuration dependent damping/diffusion in a heat-bath basically drives the motion in the absence of any active force. It is very important to note that, in the absence of state dependent damping/diffusion i.e., when the constituent particles of dimer are similar, no such sustained directed motion of the structures formed are seen although all other parameters were kept fixed. That the conservative interaction parameters are kept the same can be seen in each case in the similarity of the structures formed in the symmetry-broken as well as in the symmetry-unbroken cases. These null results in the symmetry-unbroken cases stand as the proof that there indeed is present directed transport driven by thermal fluctuations in the presence of coordinate/state dependent damping and corresponding diffusion.

The simulations done for the results of the present paper are plain Langevin dynamics with a thermal noise strength kept in consistence with the Stokes-Einstein rela-
tion. There is no so-called fluctuation-dissipation breaking force present in the models as far as the standard theory demands. Still there are directed motions characteristic to the structures formed are manifestly present whenever the constituent monomers of the dimers have an internal coordinate (state) dependent diffusivity which are not the same functions of the internal coordinate.

Let us try to understand if we call these directed motions to be the ones happening in equilibrium with the heat bath or not by looking at the momentum conservation of the bath and the system. In the context of the Langevin dynamics, ideally in the theoretical sense, it is considered that the bath can always absorb any amount of momentum without undergoing any perturbation because it is too big with infinite degrees of freedom. Therefore, the momentum conservation, in that ideal sense in the scope of the theory, exists by an assumed distribution of the opposite momentum that the system has generated being absorbed by the bath. This is the same idea that even works in the context of the active systems because the momentum generated by the collective motions there is non-trivial only when the system is not driven on average by any directed force. Therefore, even in the case of the active systems, it is tacitly assumed that the bath degrees of freedom help maintain the momentum conservation without altering the temperature of the bath because the bath is too big.

However, no real bath is that big and the idealization of the theoretical considerations underlying the Langevin dynamics would break down in real systems. Despite that, in the presence of the broken symmetry due to coordinate/state dependence of the system, thermal fluctuations will always drive such directed motions which will eventually be transient due to the perturbation of the bath to conserve the momentum. Now, on one hand, even such transient directed motions could play important role in structural transitions of the system following which the bath will stabilize through essentially non-equilibrium processes.

On the other hand, there also exists the scope for the bath periodically coming back to the equilibrium after every step of some directed motion of the system and a non-equilibrium steady state of such motions existing. However, in all such real cases, although the directed motion is associated with non-equilibrium processes of periodic equilibration of the bath, it is the bath fluctuations alone that can produce such directed motions and one does not necessarily need any extra drive on top of the bath fluctuations. This is an alternative scenario to the so far known active transport where one uses an activation force on top of the bath fluctuations.

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