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Review Paper

Self-Propelled Dynamics: Insights from Brownian motion Studies

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Abstract

Self-driven (or active) particles are capable of converting stored energy into coordinated motion. Systems of active particles are far-from-equilibrium and are studied using concepts such as the Langevin formalism, the Fokker-Planck equation, the Master equation, the Boltzmann equation. In this review, we discuss models of active matter covering systems from individual particles to collections of interacting and non-interacting ones, within the framework of active Brownian motion. First, we discuss general idea of Brownian dynamics for passive particles. Equations governing passive particle dynamics follow detailed balance and hold fluctuation-dissipation theorem (FDT). In active systems detailed balance is broken and FDT is violated. We write the corresponding Langevin equation for active particles for a minimal model and analyse the equation to study the critical dynamical behaviour such as collective organized motion, motility-induced phase separation (MIPS). We discuss how to extend these ideas to other complex systems and explore some practical applications.

Keywords: Self-driven particles, active matter, non-equilibrium systems, Langevin equation, active Brownian motion, coordinated motion, order-disorder transition.

Introduction

Active matter systems are composed of a large number of particles that propel themselves using their own energy. Each element of the active matter system are equipped with internal engines that allow them to continuously convert energy, sourced either internally or externally (ambient free energy), and enabling them to perform work[1,2]. Because of this behavior at the level of individual particles, the system exists in a non-equilibrium state. Examples of active systems mainly consist living entities and also some manmade systems like robotic swarms. They are found across a broad range of length scales, from microns to kilometer range, e.g., motor proteins, cell cytoskeleton, tissues, colloids, bacterial suspensions, bird flocks, fish schools, animal herds (Figure-1).

Systems of self-driven particles are different than the classical equilibrium systems which are well described using the notion of equilibrium statistical mechanics. Statistical mechanics is a microscopic theory that links the microscopic properties for a system of particles to macroscopic parameters based on the concept of partition functions or statistical ensembles[3-5]. Unlike passive particle systems, we do not have equation of state and well defined Hamiltonian for active matter systems.

The thermodynamic parameters like temperature, pressure, etc. cannot be obtained in a traditional manner. Active systems are divided into ‘dry’ and ‘wet’ systems based on the momentum conserving properties. In a dry active system, particles move on a solid substrate and momentum conservation is violated due to frictional drag. On the other hand in wet active systems, dynamics is momentum conserving. Generally, wet systems are formed by active particles suspended in a fluid medium. The first model of active matter (an ideal model) for the motion of self-driven particles was proposed by Vicsek et al.[6]. The model showed non-equilibrium phase transitions from disordered to ordered states as particle density increases or noise decreases[6]. This interesting phenomenon led to further theoretical and experimental development of this new area of physics.

The simplest approach to write microscopic dynamical equations for such systems is to start with the Langevin equation. In the conventional Langevin equation for passive Brownian particles, the microscopic dynamics do not conserve momentum. In dry active matter, the time evolution equations for position and momenta are modeled by extending this idea. For large-scale dynamics, the microscopic equations are coarse-grained by averaging out the fast degrees of freedom of the system.

Passive particle Brownian dynamics

We discuss the general framework of classical Brownian motion. The Ornstein-Uhlenbeck process, Brownian motion, etc. are the basic models to study the complex stochastic systems such as stock market fluctuations, biological processes, population dynamics. Many biological processes require a constant exchange of energy and hence fall in the category of active systems.

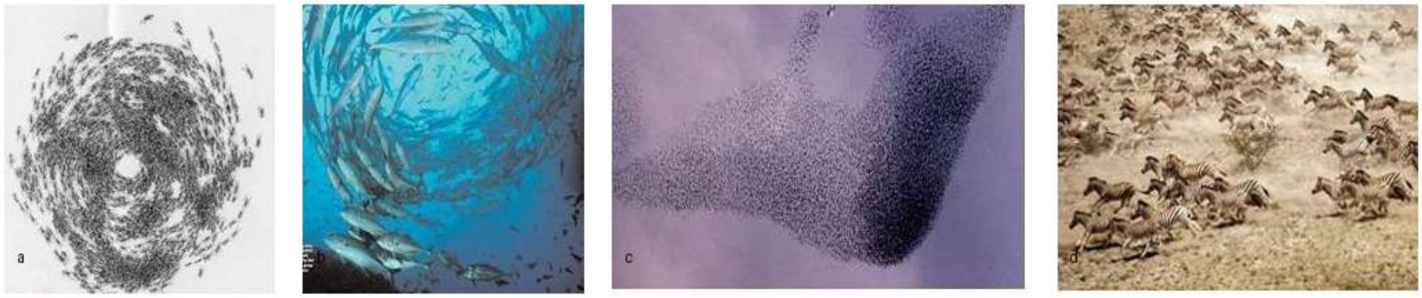

Figure-1: a) Army ants representing collective rotating motion. b) Schooling fish showing coordinated swimming. c) Bird flock illustrating natural flocking behavior. d) Collective motion of a herd of zebra[7].

Brownian motion refers to the erratic movement of a large particle suspended in a fluid. The random and irregular movement of this large particle, which we call as Brownian particle, results from constant, random collisions with nearby fluid particles. The initial theoretical framework for Brownian motion was given by Einstein and Smoluchowski, and it was later further developed by Langevin and others[8,9]. We give here detailed description of Langevin formalism of Brownian dynamics. In classical statistical mechanics, the motion of a system involves phase-space coordinates.

Translational motion: Langevin equation is the stochastic differential equation in terms of time derivative of position and velocity (momentum) variables. In order to write the Langevin equation for a Brownian particle, we assume that the mass of the Brownian particle is m, and velocity at time $t$is represented by $u(t)$. We assume that the force experienced by the Brownian particle consists of two terms. The first term is the dissipative force term that is proportional to the velocity and directed opposite to it. This term represents the deterministic part of the equation. The second term is the stochastic or random force $\xi(t)$, which results from the random collision of surrounding particles. The Langevin equation is written as:

$$\frac{dx}{dt} = u, m\frac{du}{dt} = -\zeta_0 u + \xi(t).$$

The above equation is in the simplest form in which the interaction term between particles is not considered. Interaction term is time reversible and contribute to the deterministic part. This equation is a first-order ordinary differential equation which can be solved using the ordinary rule of the Calculus.

Assuming the white Gaussian noise, we write $\langle \xi(t) \rangle = 0$ and the noise-noise correlation is given as $\langle \xi(t)\xi(t') \rangle = D\delta(t - t')$, where $D$is noise strength. Using above assumption, the average velocity of the particle is:

$$\langle u(t) \rangle = \langle u_0 \rangle e^{-\zeta_0 (t-t_0)}$$

The average velocity decays exponentially from its initial value. In thermal equilibrium, the initial velocity directions are randomly distributed, so $\langle u_0 \rangle = 0$. Therefore, $\langle u(t) \rangle = 0$ for all times, implying that in thermal equilibrium, there is no net motion for a collection of Brownian particles. The noise strength in equilibrium condition is given as $D = 2k_B T\zeta_0$.

The velocity autocorrelation function defined by $C(t, t') = \langle u(t)u(t') \rangle$, in the long time limit, assuming that the Brownian particle equilibrates at temperature T, is obtained as

$$C(t, t') = k_B T e^{-\zeta_0 |t-t'|}$$

This equation depends only on the time difference and is time translation invariant.

Mean Square Displacement (MSD) and Stokes-Einstein Relation: The root mean square (rms) displacement of the Brownian particle can be obtained by integrating the velocity correlation function with respect to time. Using the definition $u = d\,x/d\,t$:

$$\left\langle \frac{d}{dt}x(t)\frac{d}{dt'}x(t') \right\rangle = k_B T e^{-\zeta_0 |t-t'|}$$

Integrating at times t and t', the rms displacement is given as

$$\langle \Delta(t)\Delta(t') \rangle = k_B T\zeta_0^{-1}\left[t + t' - |t - t'| - 2t_0 + \zeta_0^{-1}\left(e^{-\zeta_0(t-t_0)} + e^{-\zeta_0(t'-t_0)} - e^{-\zeta_0(t'-t)} - 1\right)\right],$$

Where: $\Delta(t) = x(t) - x(t_0)$. For the equal time case $t = t'$, we obtain $\langle \Delta^2(t) \rangle = 2k_B T\zeta_0^{-1}\left[t - t_0 - \zeta_0^{-1}\left(e^{-\zeta_0(t-t_0)} - 1\right)\right]$.

There are two cases of above equation: the short time limit $\zeta_0^{-1}(t - t_0) \ll 1$and the long time limit $\zeta_0^{-1}(t - t_0) \gg 1$. For very short times , the rms displacement is linearly proportional to time and particle behaves as a free particle. In the long limit the MSD has linear dependence with time. This is called the Einstein relation. The relation between the diffusion coefficient (say) D_0 and the frictional coefficient ζ_0 is given as $D_0 = k_B T\zeta_0^{-1}$. Using Stokes' law $\zeta_0 = 6\pi r\eta_0$, where r is the radius of the Brownian particle and η_0 is the shear viscosity of the surrounding liquid we obtain diffusion coefficient as $D_0 = \frac{k_B T}{6\pi r\eta}$.

This is the Stokes-Einstein relation, which indicates that the diffusion coefficient D_0 and the viscosity η_0 are inversely proportional to each other.

Rotational Motion: Similar to translational motion one can obtain the orientational dynamics of the Brownian particle . We consider two-dimensional dynamics with director vector $\hat{e} = (cos\theta, sin\theta)$. Assuming that moment of inertia of the particle is I, rotational frictional drag ζ_θ, and stochastic torque due to collision of surrounding medium η_θ, the corresponding Langevin equation is given by

$$\frac{d\theta}{dt} = \omega, I\frac{d\omega}{dt} = -\zeta_\theta\omega + \eta_\theta(t).$$

The noise-noise correlation of the Gaussian random torque η_θ is given by
$$\langle\eta_\theta(t)\eta_\theta(t')\rangle = 2k_BT\zeta_\theta\delta(t-t').$$

The angular mean square displacement (AMSD) $\Delta_\theta(t) = \big(\theta(t) - \theta(0)\big)$ for overdamped dynamics is given by
$$\langle\Delta_\theta^2(t)\rangle = 2k_{BT}\zeta_\theta^{-1}t = 2D_\theta t,$$

where D_θ denotes the rotational diffusion coefficient which can be linked to the viscosity of the medium using the Stokes-Einstein relation.

Active particle dynamics: the active Brownian motion

In a system of active Brownian particles there is a regular flow of energy exchange and the system is out of equilibrium Thus, this kind of model is of great interest to understand non-equilibrium processes. The microscopic dynamics of active systems are not constrained by time reversal symmetry. Therefore, we need different approach than the passive particle systems to obtain macroscopic dynamics from microscopic models. Constraints like energy conservation, momentum conservation, divergence free currents in steady state , etc. can not be used to obtain closed form of dynamical equations. Many processes involving living entities such as bacterial motion (e.g., E.Coli bacteria), cellular function of animals involve net flow of energy and can be understood using the concepts of active Brownian motion studies. In active system fluctuation-dissipation relation (FDR) and standard Stokes-Einstein relation do not hold.

In the microscopic Langevin equation of active Brownian particles there is an additional self-propulsion force term which is responsible for energy input into the system. Noise force term in the equation can also play the role of energy input for a particular system. The equation can be formulated as
$$\frac{dx}{dt} = v, m\frac{dv}{dt} = F_{drag} + F_{ip} + F_{sp} + \eta_a,$$

where $F_{drag} = \zeta v$ is the frictional force term, F_{ip} denotes interaction term, F_{sp} denotes self-propulsion term and η_a is the active noise term. This is generalized equation valid for d dimensions. If we take dissipative coefficient ζ as a function of velocity like $(-\zeta_0 + \zeta_1 v^2)$ it will have the property of energy injection and dissipation[10]. The first term pump energy and the second term put restrictions to the motion. The nature of interaction potential term also play the crucial role for emergent behaviour of the system.

Next, we discuss the model of self-propelled polar disks on a substrate in two dimensions with isotropic repulsive forces and rotational noise, but no aligning interaction[11]. The microscopic equations involving translation and rotational motion in 2D for individual particle dynamics is given as
$$\frac{dx}{dt} = v_0\hat{e} + \eta_T(t); \frac{d\theta}{dt} = \eta_R,$$

where $\hat{e}$ is the orientational vector in 2D, η_T and η_R denote respectively translational and rotational Gaussian noises with noise strengths D_T and D_R. The self-propulsion speed is denoted by v_0. Following the earlier above discussed procedures the MSD is obtained as.
$$\langle\big(\Delta x(t)\big)^2\rangle = 4D_Tt + \frac{2v_0}{D_R}\left(t - \frac{1-e^{-D_Rt}}{D_R}\right)$$

This model showed ballistic behaviour at short time with $\langle\big(\Delta x(t)\big)^2\rangle \sim v_0^2t^2$ and diffusive behaviour at long times with $\langle\big(\Delta x(t)\big)^2\rangle \sim \frac{v_0^2}{D_R}t$. This system shows phase separation behaviour under variation of certain parameters such as density, self-propulsion speed[12, 13].

Conclusion

We have discussed passive Brownian dynamics followed by active Brownian motion. In passive particle motion, the system reaches at equilibrium point at some temperature T. We have obtained the conventional relations like FDT, Stokes-Einstein relation of equilibrium dynamics. We have also obtained the rotational dynamics of passive particles. Analogous Stokes-Einstein relation and FDT are discussed. Violation of these relations indicate far from equilibrium systems like active matter, glassy systems, boundary driven systems, etc.

In active Brownian dynamics key terms in the Langevin equations are self-propulsion term and active noise term. Due to non equilibrium nature of the system, time evolution equations do not give rise to conventional relations. We get effective diffusion coefficient. We have seen how diffusion takes place at short and long time limit respectively. Exact temperature and pressure relations cannot be obtained. Applications of active dynamics are useful in many areas, such as medical science[14], material science, navigation technology and traffic dynamics[15]. Study of these kind of systems provides new dimensions for non-equilibrium statistical physics.

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