Nonequilibrium dynamics and thermodynamics of some single-particle activity-induced diffusive systems

Abstract

In the mesoscopic world, diffusion is a ubiquitous process and it is usually explained by the Einstein's theory of Brownian motion (BM). However, in the biological systems, some peculiar dynamical behaviors are observed as opposed to those of the BM [1,2]. Such characteristics can be understood by considering that apart from the thermal noise, the system is subjected to an additional noise called active noise stemming from some active processes such as ATP hydrolysis. Due to the presence of active noise, the system is driven out of equilibrium as it is manifested by the breakdown of the conventional fluctuation-dissipation relation (FDR).

In the first part of my thesis (Chapter 1- 5), we study two activity-induced diffusive systems - (i) self-propelled particle and (ii) passive colloidal particle in the active surroundings [3]. The dynamics of a self-propelled particle is conceived through the run-and-tumble particle (RTP) model in which the active noise is taken as dichotomous (telegraphic) noise. By employing the phase-space path integral (PSPI) technique, we find that unlike free Brownian motion, the distributions at early and intermediate times are double-peaked, as has been observed experimentally [4]. On confining them in a harmonic potential, the distribution is often found to be concentrated near the boundaries. This is the trait of RTPs such as bacteria, Janus particles, as supported by many theoretical calculations and experimental evidences [5]. Another problem we deal with is the diffusive motion of a passive particle in a bath containing active particles such as bacteria, motor proteins, etc. By modelling the active bath by Gaussian colored noise (GCN), we find that the distribution is always Gaussian with an enhanced diffusivity. Similar traits have been observed in the diffusion processes of colloids in a low-dense bacterial solution [1, 6]. In many recent experiments on the dynamics of colloids inside a living cell, it has been found that the distribution has a long exponential tail [2]. By taking the active noise as Poissonian white and Poissonian colored noise (PWN and PCN), we explain the results. Also, many transient behaviors of these models are explored theoretically [3].

In the second part of my thesis (Chapter 6), we theoretically study the first passage problem of a particle which diffuses with a diffusion constant which switches between two states [7]. This model is used to investigate the target search by protein molecules along a DNA chain. By computing the survival probability, the average rate and the absorption rate, we find that (i) the particle has a better chance of survival in the presence of sinks for the switching diffusion compared to a system having single diffusivity (normal case), and (ii) the absorption rate is comparatively enhanced for the switching case at the intermediate timescale. In the long-time limit, the rate in both switching and normal diffusion are equal. We also investigate the impact of different parameters such as initial positions, Poisson rates, the strength of diffusivity. This study may be helpful to find the suitable conditions for the optimal search strategy.

In the final part of my thesis (Chapter 7-9), we investigate the thermodynamic properties of a passive colloid diffusing in an active bath. We study work fluctuations in two different active baths, namely GCN and PWN baths for two different protocols [8]. Further we investigate the fluctuation relations (FR) to find that the conventional FRs of work with the ambient temperature does not hold in the transient period, as reported earlier [9], but at the steady state a certain kind of FR emerges in which the ambient temperature is replaced with an effective temperature. This is valid for both the models, and it is in sync with the one obtained experimentally by Maggi *et. al.* [9]. Also, in GCN model, we establish an FR analogous to the Jarzynski equality (JE) following the Hatano-Sasa formalism. Another important quantity we study is the heat fluctuations for a trapped Brownian particle in an active bath [10]. The GCN and PWN models are used separately to design the active bath. For both cases, the heat distribution is computed to find that there is a net heat flux towards the particle, and it is substantiated by an FR at the steady state. Then we compute the total entropy production which justifies the second law of thermodynamics. Our system can be used to design mesoscopic heat engine.

References:

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