

Effective single particle theory for active particles using local density fluctuations

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Abstract – We characterize the dynamic non-equilibrium steady state behavior of active particles using density fluctuations in the system. We analyze the effective local density around a particle in the steady state and numerically calculate its mean, variance and auto-correlation. Thus, using local density and its statistical properties as a temporally correlated stochastic variable, we develop an effective single-particle theoretical model and analytically derive an expression for the particle’s diffusivity as a function of the global packing density in the system. Our theory accurately predicts the transport properties of an active particle, validated against numerical simulations. Unlike mean-field theory, which fails at high packing densities due to significant density fluctuations from dynamic cluster formation, our model remains effective across all densities. It also captures the well-known phase transition beyond a critical packing density. The key novelty of our model lies in the introduction of a stochastic local density field, which encapsulates the effect of steric interactions on an active particle and helps predict single-particle behavior in a collection—a feature often absent in standard active matter models. This approach could be useful in experimental setups where fluctuations in local density around a tagged particle are measurable.

Introduction- Active matter constitutes a distinct class of non-equilibrium systems that are composed of particles that consume energy from their surroundings and convert it into motion or exert mechanical forces [1–6]. It encompasses a wide range of examples, from the biological realm, including microswimmers such as E.Coli bacteria [7], collective behaviors observed in groups of animals such as fish schools [8] and bird flocks [9], as well as artificial microswimmers, colloidal suspensions, and robots. On an individual particle level, because of the constant flux of energy, an active particle is in a perpetual far-from-equilibrium state. In such a non-equilibrium state, the particle produces net entropy while breaking the usual equilibrium conditions of detailed balance and time-reversal symmetry. Thus, activity of a single particle adds complexity in its motion, and hence its motion is studied through frameworks of non-equilibrium statistical physics.

Another layer of complexity in behavior of active matter systems is added when active particles are in a collection, and the individually out-of-equilibrium particles interact to display emergent steady-state phenomena like novel phase transitions, long-range ordering, giant number fluctuations, collective motion and self-organization,

which are not observed in equilibrium systems [10–16]. There is a gap in understanding the dynamic behavior of active matter systems in non-equilibrium steady states specific to its effect on a single particle. In this study, we take a top-down approach, first characterizing the steady-state behavior of the system using a stochastic local density variable in numerical simulations, and then using it to theoretically calculate the effective dynamics of a single particle. We use active Brownian particles [17–23], which are self-propelled disk-shaped particles that move at constant speed, maintaining their direction for some time before reorientation due to thermal fluctuations. This system exhibits motility-induced phase separation (MIPS) above a threshold packing density, characterized by the dynamic formation and dissolution of macroscopic clusters. We theoretically model dynamic cluster formation and dissolution by introducing a local density variable. Starting with an analysis of local density fluctuations around a tagged particle in simulations, we proceed to calculate effective local density fluctuations by averaging over all particles and ensembles. In the steady state, we numerically compute key statistical properties, such as mean, variance, and temporal auto-correlation of local density, which remain constant, characterizing it as a sta-