Metastability and Phase Coexistence in Active Brownian Systems

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Soft Active Matter is a collection of systems that are intrinsically out-of-equilibrium. A system of self-propelled particles whose orientation vector is subject to a difusion process breaks time-reversal symmetry on the local scale once we introduce excluded volume interactions, and thus breaks detailed valance. These systems are mantained out-of-equilibrium in the presence of a source of energy such as chemical products; free energy is converted into momentum. To model systems of microswimmers (bacteria or Janus colloids), midges, and, lambs the Active Brownian Particle model is a good choice.

Active Brownian Particles (ABP) exhibit a density phase separation, the so called Motility Induced Phase Separation (MIPS)[1]. The combination of prupulsion and repulsion in ABP systems gives an emmergent relation for the local mean velocity as a function of the local mean density; it decreases linearly. The accumulation of particles at slow regions of the space may trigger, as a function of proupulsion and total density, a phase coexistence between a macroscopic high-density aggregate and a dilute gas.

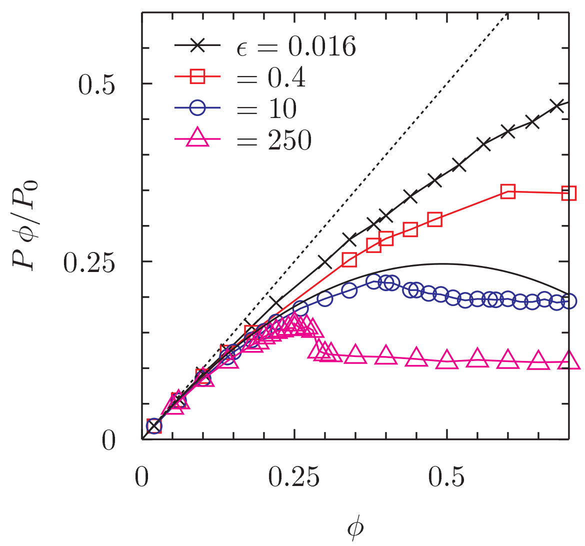

Figure 1: Pressure of a system of ABP with Periodic Boundary Conditions (PBC) at a fixed value of the propulsion, $Pe = 30$. Different colors label systems with different rigidities in the repulsive potential. A pressure drop is found for $\epsilon > 1$ at the vicinity of the separation.

Extending thermodynamics to such systems is not trivial and the most intuitive thermodynamic variable to extend is pressure[2]. Following the pressure across MIPS, a pressure drop has recently been reported that indicates MIPS but it is above the coexistence density [3, 4]. This pressure drop is depicted in Figure 1. Contrary to some works, we claim that this pressure drop is not a characteristic feature of this phase separation but an effect of sampling in a metastable region of the coexistence.

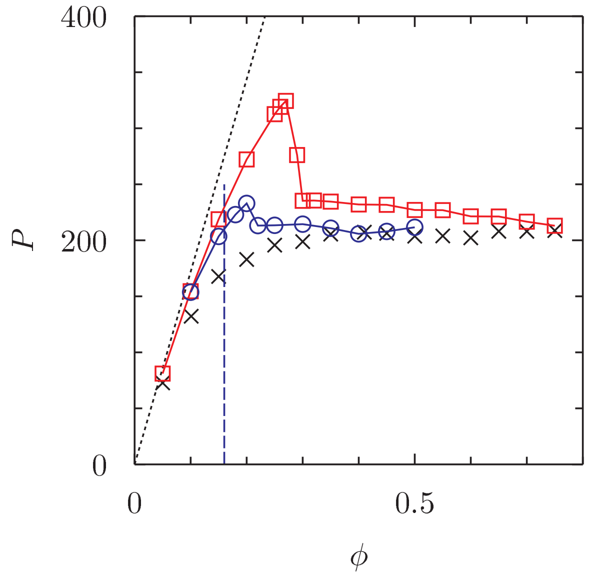

Figure 2: Active Pressure following three different preparations. In Red we prepare homogenious initial conditions and measure the steady pressure. In Blue we quench a phase separated system into a lower density. In Black cosses a the system contains a hard wall. We report an hysteresis loop

The preparation of the system is usually performed by randomly distributing particles in the simulation box. We can also start from an already separated configuration and then expand the simulation box to reach the desired densityOnce the system reaches a steady state; pressure is measured. These two procedures have been implemented and the results are shown in Figure 2.

Simulations show a hysteresis loop in the pressure; the system stays separated at lower densities than ever reported. By quenching a phase separated system to lower densities we explore MIPS by means of the active pressure at all densities and identify the metastability region.

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