The equation of state of Active Brownian Hard-Disks

Demian Levis[1], Joan Codina[1] and Ignacio Pagonabarraga[1]
[1]Departament de Física de la Matèria Condensada, Universitat de Barcelona, Martí i Franquès, E08028 Barcelona, Spain

Active matter systems made of self-propelled particles can be found across a broad range of length scales, both in living and synthetic man-made systems, like bacteria suspensions, animal groups or artificial colloidal swimmers [1]. The fundamental difference between active systems and standard 'passive' matter made of thermally agitated constituents, is that the microscopic dissipative dynamics of the former breaks detailed balance and, as such, evolves out-of-equilibrium. The out-of-equilibrium nature of active matter manifests strikingly in the presence of interactions. Self-propelled spherical particles accumulate in regions of space where their velocity decreases as a consequence of collisions. At high enough densities and activities a purely Motility-Induced Phase Separation (MIPS) takes place, leading to the coexistence of an active low density gas with a high density, solid-like phase solely sustained by activity. This out-of-equilibrium transition is reminiscent of equilibrium liquid-gas de-mixing. It is thus tempting to try to extend the thermodynamic description of first order phase transitions in terms of, for instance, equations of state, to ABPs. However, this poses several fundamental difficulties since no thermodynamic variable is, in principle, well defined in this context.

Much work has been recently done to extend the notion of pressure for this systems, and therefore study their equation of state, both from a theoretical and experimental perspective[2, 3]. However, the construction of a general thermodynamic framework is still in progress and the nature of the pressure across MIPS is a matter of debate. Several works have found an abrupt pressure drop at the vicinity of MIPS, occurring at densities well above the coexistence ones, and have argued that it constitutes a distinctive feature of this transition [4]. A pressure loop generically appears in constant-density simulations of equilibrium systems showing phase coexistence , an effect that can be suppressed by the Maxwell construction to extract the behaviour of the system in the thermodynamic limit. However, this construction is violated for ABP and there is no direct way to understand the phase diagram of the system from the simulated equations of state. There are some inconsistencies in the simulation results reported so far and a proper interpretation of the equations of state obtained so far is still lacking.

We show here that the equations of state of ABP across MIPS are consistent with the first-order phase transition scenario and allow to characterize its phase behaviour, providing a consistent thermodynamic interpretation of the numerical data. By changing the preparation protocol and the topology of the system, we bring out the existence of a metastability region : an *hysteresis* around the coexistence pressure is found in the equations of state as the system is quenched to the coexistence region from different states. By analyzing simultaneously periodic and confined systems, we show that the pressure drop and the invariance of the first virial coefficient found in previous simulation studies is due to the presence of a large nucleation barrier. This can be easily bypassed by initializing the system in the coexistence region or including a nucleation core. Then one can generate numerically a motility induced phase separated state arbitrarily close to the binodal, i.e. at densities well below those previously reported. To show these results, we perform constant-density simulationsof Active Brownian Hard-Disks and ABP interacting with a WCA potential.

We apply a recently developed extension of classical nucleation theory for active systems [5] to justify our interpretation. We show that the presence of walls facilitates nucleation because of wetting and allows to recover the equality of pressure at coexistence. We discuss to what extent equilibrium-like ideas can be useful to describe active systems and how the understanding of the motility induced nucleation process can be used to control aggregation in microswimmer suspensions.

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