Interface Fluctuations and Intrinsic Profiles in Mobility Induced Phase Separation

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We analyse the interfacial line in two dimensions (2D) Mobility Induced Phase Separation (MIPS) of active Brownian particles, with Lennard-Jones (LJ) interactions, in the high activity regime, when the dynamics of the particles is fully dominated by a high active force, with random diffusive changes of the activity direction in each particle, but with a persistence time which becomes longer than the collision time in the dense phase of the MIPS (see general references in [1]). Simulations of a dense slab, self-maintained in contact with a low density gas, are analysed to identify the instantaneous shape of the interfacial lines, at the two edges of the slab. The accumulated statistics for the Fourier components of the lines shows independent Gaussian probabilities which may be interpreted as those of an effective thermal equilibrium interface, and used to get effective values of the line tension and bending modulus for the MIPS system.

In 2D the width of the interfacial fluctuations grows as the square root of the line length, much faster than the logarithmic effect of the capillary waves in a three dimensional liquid surface. Large MIPS simulations are required to get a good representation of dense slab, with long range structures associated to hexatic order [1], and that large size of the simulations implies a severe lost of detail in the structure of the interfacial region, when represented by the mean profiles of the density and any other property. The identification of the instantaneous interfacial lines allows to calculate intrinsic profiles for the density, the particle polarization and the interaction forces, eliminating the local wandering of the interface that smooths the mean density profile and blurs out the details of the interfacial region. The intrinsic profiles are independent of the system size (for large enough systems) and they give important clues on the physical mechanisms for the MIPS.

In normal (thermal equilibrium) liquid-vapour surfaces the intrinsic density profiles show a dense structured liquid right from the inner edge of the instantaneous interface, but in the MIPS intrinsic profiles the density raises smoothly over a thick interfacial region of $15-20$ particle diameters. Moreover, the shape of the intrinsic profiles is surprisingly similar over a large range of the active force, showing a perfect scaling with the density difference between the 2D quasi-crystal a the center of slab and the low density of the gas phase. The intrinsic density profiles for the local polarization of the particles and the LJ-interaction force acting on each particle show that this thick region (at the inner side of the dense slab) contains the main contribution to the 'rectification' of the active force that is at the core of the MIPS. The randomly orientation of the active force is usually interpreted as an 'exotic' kinetic effect, that shakes the particles in a different way than a thermal equilibrium, but which does not act (in average) as an external potential able to produce a pressure gradient across the interface. This view has been recently challenged [2] by Omar et al. pointing that, when the persistence time of the active force orientation becomes larger than the mean free path of the particles, the (null) averaged polarization of each particle may be 'locally rectified', i.e. it may become a non zero mean local polarization of the 'particles at a given position' at the interface. That mean local polarization implies that the (externally applied) 'active force' acts as a stationary external potential across the interface, producing a pressure difference between the two coexisting phases. The intrinsic analysis presented here not only supports that view, but it also characterizes the inner side of the interface, i.e. the thick region where the intrinsic density profile raises smoothly, as the main source for the active force rectification, and associates it to the distribution of 2D-crystal defects, as lines of dislocations anchored at the source provided by the interface.

The observed scaling of the intrinsic density profiles matches with the view that the universality class that described the MIPS (over a very broad range of the activity force) is not 'liquid-vapour like', based on a scaling length that diverges at the critical point. Instead the scaling is based on the 2D quasi-crystal lattice parameter, that sets the density in the dense slab and that reflects the balance between the particle (repulsive) interactions and the pressure generated by the active force (kinetic pressure of the gas, plus rectification effects across the interface). The closing dome, at the lower values of the activity force that produce MIPS, occurs very close to the melting of the hexatic structure in the dense slab, which implies the breaking of the 'high-activity' regime that cover most of the usual range over which MIPS has been studied.

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