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Phase behavior and topological defects of active Brownian particles in two dimensions

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From large-scale Molecular Dynamics simulations, we performed a complete analysis of local hexatic parameter, local density ad out-of-equilibrium equation of state of self-propelled hard disks in two spatial dimensions. We established the complete phase diagram of the model. The equilibrium melting follows a mixed scenario with first-order liquid-hexatic transition and BKT hexatic-solid one. This scenario is maintained at small activities, with coexistence between active liquid and hexatic order. As activity increases, the emergence of hexatic and solid order is shifted towards higher densities. Above a critical activity and for a certain range of packing fractions, the system undergoes motility-induced phase separation and demixes into low and high density phases; the latter can be either disordered (liquid) or ordered (hexatic or solid) depending on the activity [1].

We also provide a quantitative analysis of all kinds of topological defects present in 2D passive and active repulsive disk systems. We show that the solid-hexatic melting is driven by the unbinding of dislocations, and dissociation of disclinations is present as soon as the liquid phase appears. These two processes are in agreement with the two defects-unbinding mechanisms predicted within the Halperin-Nelson theory of melting. Concerning the hexatic-liquid melting, we observe on top that extended clusters of defects largely dominate over the point defects. Such defect clusters percolate at the hexatic-liquid transition in continuous cases or within the coexistence region in discontinuous ones, and their form gets more ramified for increasing activity [2].

[1] PD, D. Levis, A. Suma, L.F. Cugliandolo, G. Gonnella, I. Pagonabarraga. **Full Phase Diagram of Active Brownian Disks: From Melting to Motility-Induced Phase Separation**. Phys. Rev. Lett., 121, (2018).

[2] PD, D. Levis, L.F. Cugliandolo, G. Gonnella, I. Pagonabarraga. **Clustering of topological defects in two-dimensional melting of active and passive disks**. arXiv:1911.06366 (2019).

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