Melting transition and phase diagram of 2d active hard disks and dumbbells

Pasquale Digregorio [1], Leticia F. Cugliandolo [2], Giuseppe Gonnella [1], Demian Levis [3,4], Ignacio Pagonabarraga [3,4], Antonio Suma [5,6]

[1] *Dipartimento di Fisica, Università degli Studi di Bari "Aldo Moro" and INFN, Sezione di Bari, via Amendola 173, Bari, I-70126, Italy*
[2] *Sorbonne Université, Laboratoire de Physique Théorique et Hautes Energies, CNRS UMR 7589, 4 Place Jussieu, 75252 Paris Cedex 05, France*
[3] *CECAM Centre Européeen de Calcul Atomique et Moléculaire, Ecole Polytechnique Fédérale de Lausanne, Batochimie, Avenue Forel 2, 1015 Lausanne, Switzerland*
[4] *UBICS University of Barcelona Institute of Complex Systems, Martí i Franquès 1, E08028 Barcelona, Spain*
[5] *SISSA - Scuola Internazionale Superiore di Studi Avanzati, Via Bonomea 265, 34136 Trieste, Italy*
[6] *Institute for Computational Molecular Science, Temple University, Philadelphia, PA 19122, USA*

Active materials are out-of-equilibrium systems in which the dynamics of their elements break detailed balance. Examples can be found in living systems, e.g. the collective motion of large animal groups, bacteria swarming, as well as in synthetic ones, like self-propelled grains or self-catalytic colloidal suspensions. Despite such diversity, the emergence of activity-induced collective behavior is captured by minimal models that yield accurate descriptions on their universal character. A key example is the Active Brownian Particles (ABP) model which considers spherical self-propelled particles with only excluded volume interactions. Active dumbbell model is the most simple extension of ABP for active bi-atomic rigid molecules.

Although active particles can in principle move in 3D, in most experimental set-ups they are confined to 2D. Melting in 2D is a fundamental problem that has remained elusive despite decades of intensive research. Only recently, numerical simulations [*] and experiments on colloidal monolayers indicate that melting of passive hard-disks takes place in two steps: as the packing fraction is increased, a first-order transition between the liquid and hexatic phases occurs, followed by a continuous Berezinskii-Kosterlitz-Thouless transition between the hexatic and the solid. Liquid and hexatic phases coexist close to the liquid phase.

We implemented a velocity-Verlet alghoritm in the open source software Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS), to efficiently parallelize the numerical integration of the equation of motion for both disks and dumbbells. Simulations ran with $N = 256^2$ particles, scanning almost the entire parameter space over packing fraction and activity. We also explored inite size effects, simulating systems up to 512^2 particles.

We established the complete phase diagram of self-propelled hard disks and dumbbells in two spatial dimensions from the statistics of local order parameters. For the disks we also took advantage of a careful comparison among the equation of state of the system, measured thanks to a virial approach, spacial correlations of order parameters and distributions of local quantities (local density and local hexatic parameter) in order to examine in depth the transition scenario.
We found two different pictures for the two cases considered [†,‡]. The equilibrium melting scenario is maintained at small activities for the disks, with coexistence between active liquid and hexatic order, followed by a proper hexatic phase and a further transition to an active solid. 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 MIPS and demixes into low and high density phases. For dumbbells there is a macroscopic coexistence between regions with hexatic order and regions in the liquid or gas phase over a finite interval of packing fractions. In the passive limit, this interval remains finite, similar to what has been found for the disks, but, differently from them, we didn't find discontinuous behavior upon increasing activity from the passive limit.

* E. Bernard and W. Krauth, *Phys. Rev. Lett*. **107**, 155704 (2011)
† L. F. Cugliandolo, P. Digregorio, G. Gonnella, and A. Suma, *Phys. Rev. Lett*. **119**, 268002 (2017)
‡ P. Digregorio, D. Levis, A. Suma, L. F. Cugliandolo, G. Gonnella, I. Pagonabarraga, *arXiv* (2018)