Liquid-Hexatic-Solid phases in active Brownian particles determined by stochastic birth-death dynamics

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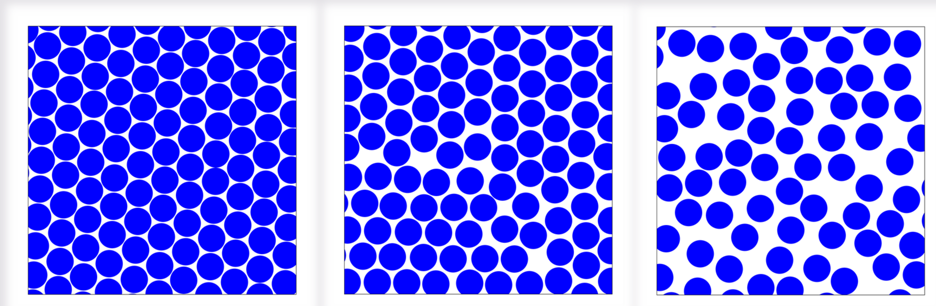
Abstract

We study the structural phases of a system of active particles[1] undergoing Brownian motion (known as active Brownian particles (ABP)) subject to volume exclusion[2]. As a new biologically-motivated ingredient we introduce stochastic reproduction and removal processes.

The number of particles in the system at long times depends on the demographic rates, and on the activity parameter. Thus, as these birth/death rates are varied we find liquid, hexatic or solid phases. As a minimal biologically motivated model considering individual size, movement and replication/birth dynamics, our results can be relevant for wound healing or tissue formation.

Phases

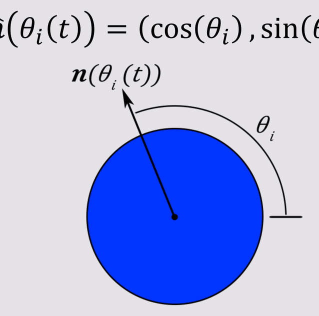


Langevin equation (Hard-core + Activity)

$$\dot{x}_i(t) = \overbrace{-\sum_{j\neq i}^{N} \nabla V(\boldsymbol{x}_i - \boldsymbol{x}_j)}^{Interaction} + \overbrace{v_0\, \hat{\boldsymbol{n}}(\theta_i(t))}^{Active\ motion} + \overbrace{\sqrt{2D}\, \boldsymbol{\xi}_i(t)}^{White\ Noise}$$

$$\dot{\theta}_i(t) = \sqrt{2D_r}\xi_i^r(t)$$

$$\hat{\boldsymbol{n}}(\theta_i(t)) = (\cos(\theta_i), \sin(\theta_i))$$



We will consider that the particles have a size, therefore, the interaction is via a hard-core potential, so that two particles cannot overlap. For this we will use the truncated **Lennard-Jones potential** (also known as Weeks-Chandler-Anderson potential).

$$V(r) = \begin{cases} 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] + \varepsilon & r \leq 2^{1/6}\sigma \\ 0 & r \geq 2^{1/6}\sigma \end{cases}$$

* *σ is the diameter of the particles*

The activity is introduced via a self-propulsion force $F_i^{act} = v_0 n(\theta_i)$, of a constant modulus v_0 and with direction given by the unit vector $n(\theta_i)$.

Demographic events

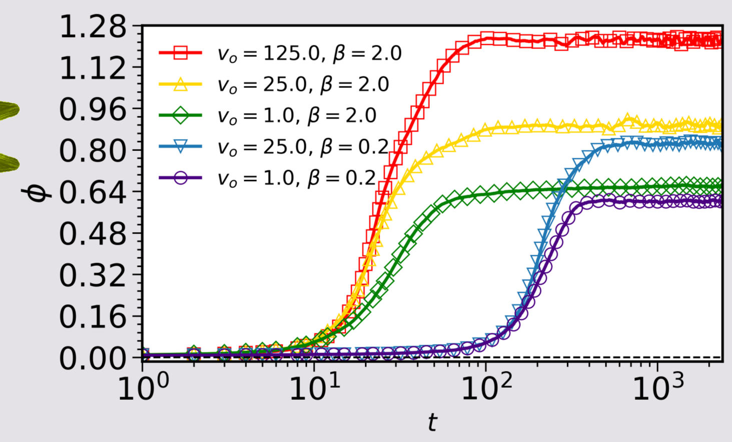
The birth-death dynamics[3] (randomly) are implemented via a **Gillespie algorithm.**

- **Death events** occur through a Poisson process with constant per-capita removal rate $\boldsymbol{\delta}$. The corresponding particle is then simply removed from the system.
- **Birth events** are more elaborate. Potential birth events are triggered with per-capita rate $\boldsymbol{\beta}$, an existing particle is selected for potential reproduction. However, the birth event can only go ahead if there is room for the offspring. The new particles are placed at a distance σ from the parent.

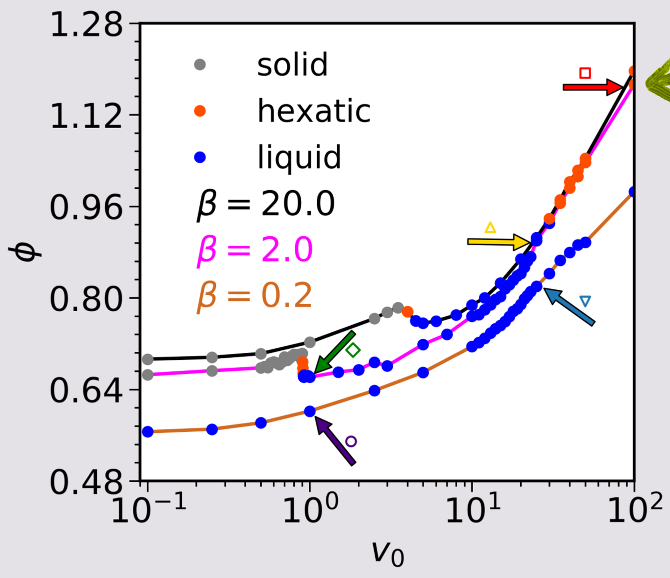
If placing the offspring there does not lead to any overlap with any existing particle, then the birth event completes. If there is overlap, then a new potential position is chosen at random from the remaining possible positions until all positions have been exhausted. In this latter case the reproduction event does not go ahead, and the simulation continues.

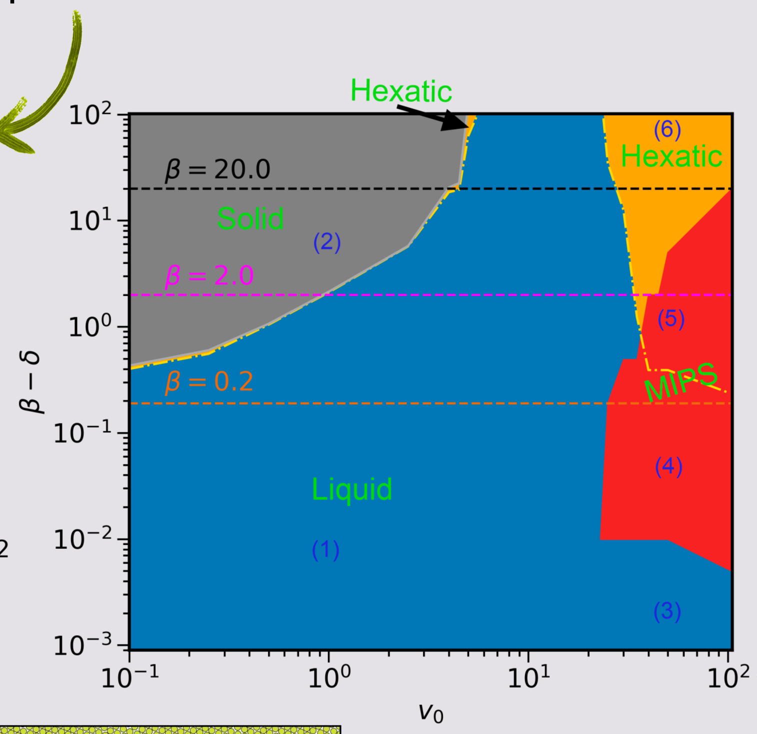
Results

- When the value of β increases, keeping all other parameters fixed, the packing fraction increases.

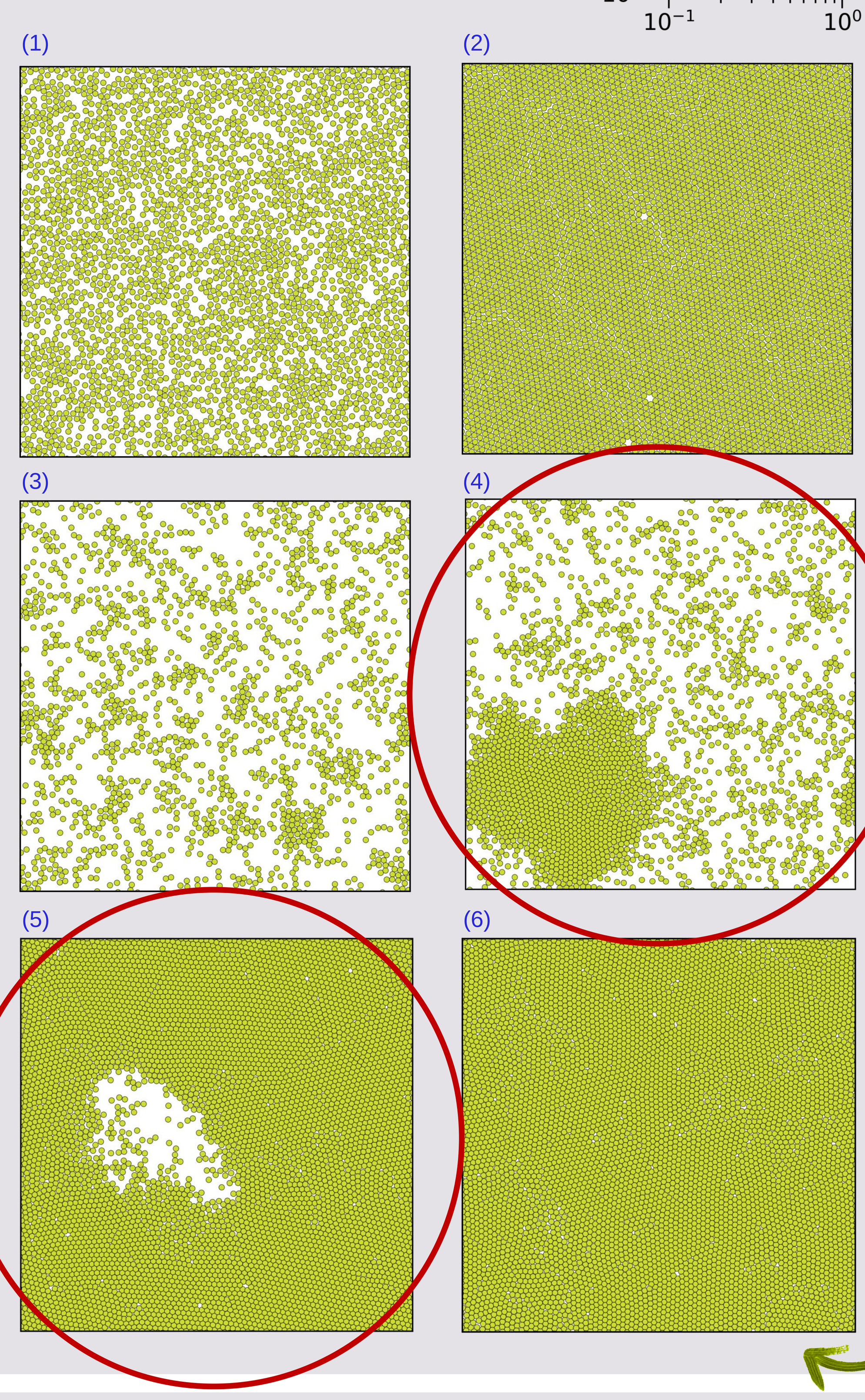


- On the other hand, an increased activity typically leads to a higher number of particles. The reason for this is that when the activity is high enough the particles may penetrate the Lennard-Jones potential and overlap. Then there is more room for self-replication.

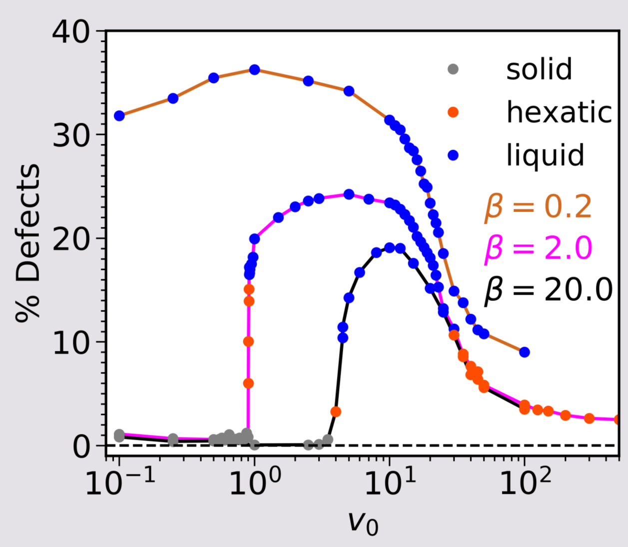




- In the regime of small activity ($v_0 < 5$), this is dominated by thermal fluctuations. Since self-propulsion plays the role of an effective temperature, the larger v_0 liquid-hexatic and hexatic-solid transitions are shifted for larger density (or lower temperature). In our case, this translates into a larger birth rate.
- Compared to the case without demography, we observe a hexatic phase after a large range of v0 values where the liquid phase is the only present one.



- For large values of v_0 we observe MIPS[4] (Motility-induced phase separation). In this regime, the system has different regions, one more ordered and dense, corresponding to the hexatic phase, and another more disordered and dilute, corresponding to the liquid phase.
- We observe a non-monotonic behavior of the number of defects with v0. For low values of v_0, the activity acts an effective temperature. When it increases the system becomes more disordered, with more defects. For large values, activity induces particle aggregation. These clusters are quite ordered due to their high density which is enhanced by birth events. When clusters occupy the whole system, the system becomes ordered returning to the hexatic phase.
- Different configurations of v_0 and β with fixed δ. These configurations are marked in the phase diagram with the same number of each figure. In the two systems presenting MIPS, we can see in a first one (4) where the cluster is small compared to the system, to a second configuration (5), where the cluster occupies almost the whole system.



Conclusions

- ✓ Long-time packing fraction depends on the demographic rates and on activity and thus these determine the structural phases.
- ✓ At difference with standard ABP system, for large activity values, the hexatic phase dominates, reflecting the greater presence of defects due to the combined effect of demographic events and activity.
- ✓ Future extensions of this work should consider more complex biological ingredients, like different size and shape for the particles, other interactions, confinement or competition for resources, but also some other types of movement like run and tumble dynamics and Levy-like flights.

Acknowledgments

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