Active Cluster Crystals with repulsive potentials

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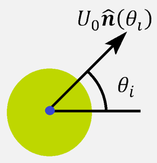
Abstract

We study numerically two-dimensional active cluster crystals using two different repulsive soft-core potentials. Cluster crystals are solids in which the unit cell is occupied by an aggregate of particles. This aggregation is a first step towards the formation of patterns. We analyze two different models of active dynamics: active Brownian particles and Ornstein-Uhlenbeck particles with two different potentials. We show a tendency of particles to aggregate depending on the parameters. To compare them, we use the radial distribution function which helps to analyze the distribution of the particles inside a single cluster.

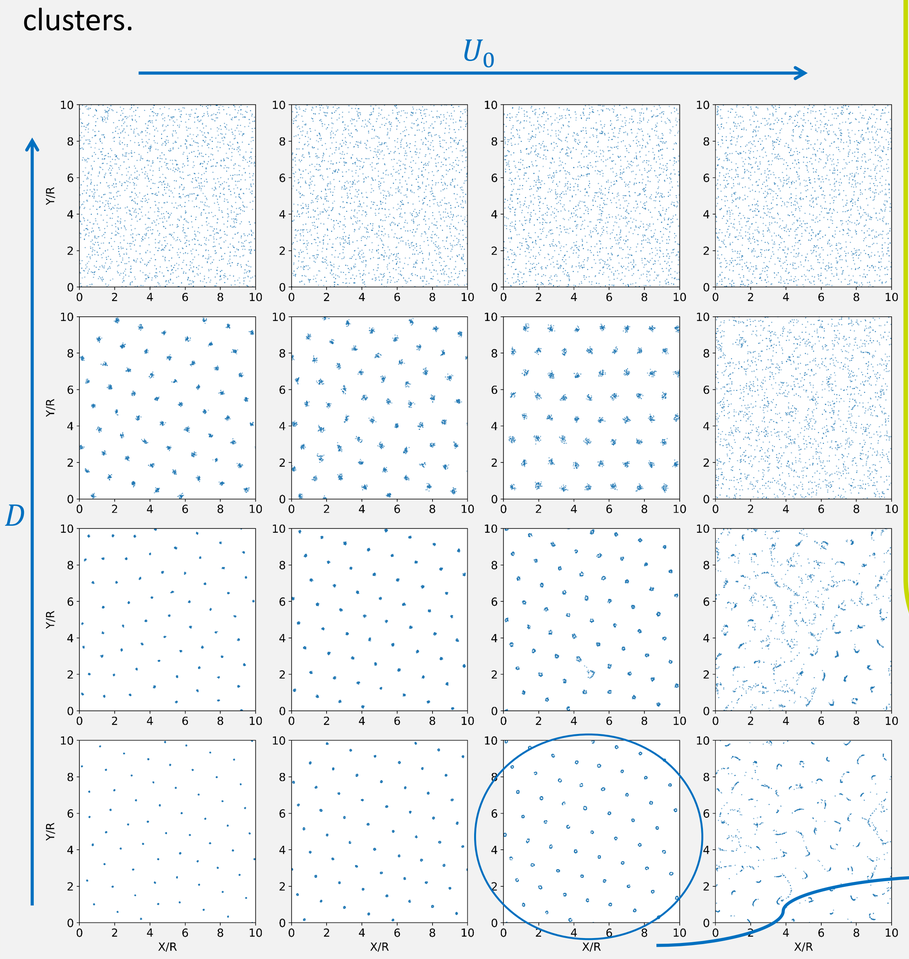
Active Brownian Particles (ABP)

$$\dot{\boldsymbol{x}}_{\boldsymbol{i}}(t) = \overbrace{-\sum_{j\neq i}\nabla V(\boldsymbol{x}_{\boldsymbol{i}}-\boldsymbol{x}_{\boldsymbol{j}})}^{Interaction} + \overbrace{\sqrt{2D}\boldsymbol{\xi}_{\boldsymbol{i}}(t)}^{White\ Noise} + \overbrace{U_0\hat{\boldsymbol{n}}(\theta_i(t))}^{Active\ motion} \qquad \hat{\boldsymbol{n}}(\theta_i) = (\cos(\theta_i), \sin(\theta_i))$$

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



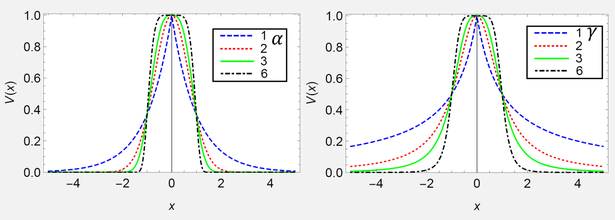
In the ABP model, the module of the active motion is constant and only change the direction in time. We observe that decreasing D we can go from a homogenous distribution to a distribution where the particles aggregate. On the other hand, increasing the value of U_0 the particles form ring shaped clusters.



Interaction Potential

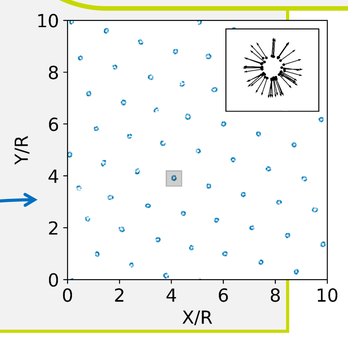
$$\boldsymbol{GEM-\alpha} \qquad V(\boldsymbol{x}) = \varepsilon \exp\left(-\left|\frac{\boldsymbol{x}}{R}\right|^{\alpha}\right)$$

$$\boldsymbol{Bosonic} \qquad V(\boldsymbol{x}) = \frac{\varepsilon}{1+\left|\frac{\boldsymbol{x}}{R}\right|^{\gamma}}$$



All the screenshots are made with the $GEM-3$ ($\alpha = 3$) . The important characteristic of these potentials is that they have negative values of the Fourier transform. This is necessary for the formation of clusters.

We obtain the same results for both potentials. The differences are quantitative and not qualitative.



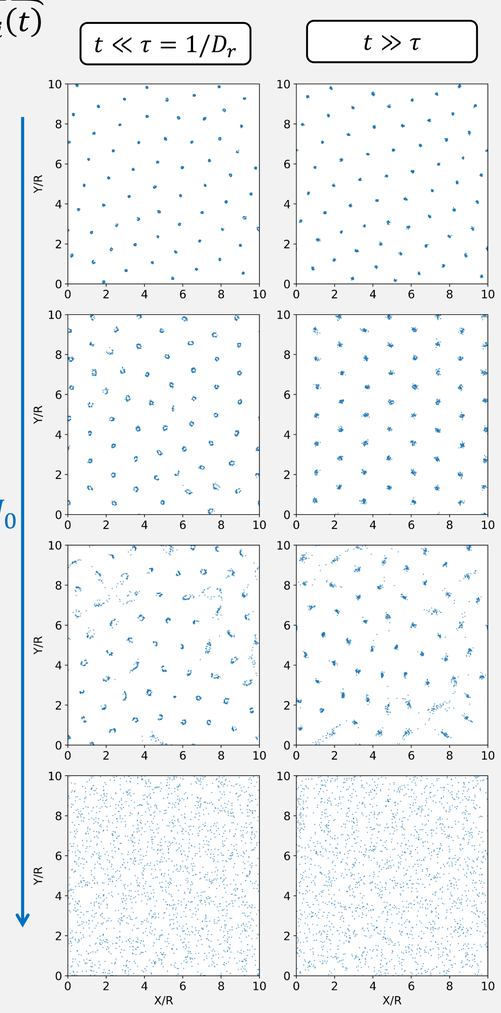
Active Ornstein-Uhlenbeck Particles (AOUP)

$$\dot{\boldsymbol{x}}_{\boldsymbol{i}}(t) = \overbrace{-\sum_{j\neq i}\nabla V(\boldsymbol{x}_{\boldsymbol{i}}-\boldsymbol{x}_{\boldsymbol{j}})}^{Interaction} + \overbrace{\sqrt{2D}\boldsymbol{\xi}_{\boldsymbol{i}}(t)}^{White\ Noise} + \overbrace{\boldsymbol{u}_{\boldsymbol{i}}(t)}^{Active\ motion}$$

$$\dot{\boldsymbol{u}}_{\boldsymbol{i}}(t) = -D_r\boldsymbol{u}_{\boldsymbol{i}}(t) + \sqrt{D_r U_o^2}\ \boldsymbol{\chi}_{\boldsymbol{i}}(t)$$

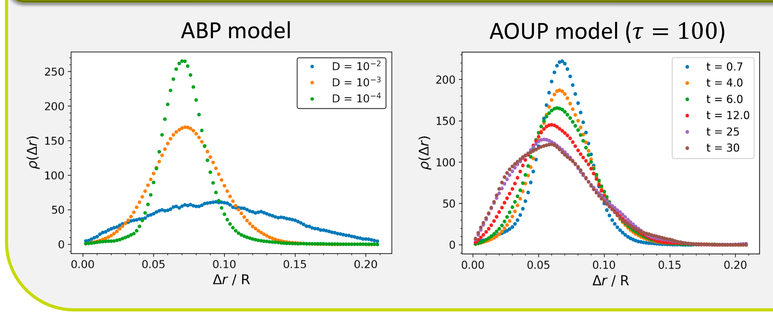
For small times ($t \ll \tau$), the particles behave as ABP, where the clusters have a ring shape within the regime where they are formed.

For large times ($t \gg \tau$), the rings disappear and the interior of the ring fills slowly behaving as a passive Brownian particle. This is due to the decorrelation with the initial condition, where all the particles have the same velocity.



The AOUP model differs from the ABP by the way of defining the active motion. It follows a Ornstein-Uhlenbeck process, where the module of the velocity is not constant in time. Although the velocity vector is different in both models, the regime where the clusters are formed is the same, it only depends on the potential.

Radial Distribution Function (RDF)



- To analyze how change the cluster, we perform the RDF whose analyze the distribution of the particles inside a cluster. We average over all the particles without differences in which cluster there are.
- As expected, if we increase the value of D the particles stay more dispersed and the peak becomes smaller and wider. Changing the intensity of the active motion (U_0), the cluster size doesn't change until the cluster is filled, where it follows a power law.
- In the AOUP model, the time until the rings are filled is $\sim\tau/4$ and to reach the steady state is $\sim\tau/2$.

Conclusions

In this work we studied the differences between the ABP and the AOUP model for active repulsive particles. As we already knew within a range of parameters, the particles were periodically located despite the repulsion between them. For active particles, we observed that they aggregate in a ring-shaped clusters that disappears for a large times in the AOUP model. This phenomena is produced because of the non-constancy of the active motion vector module.

Acknowledgments

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References

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[2] J.-B. Delfau, C. López, and E. Hernández-García, "Active cluster crystals," New Journal of Physics, vol. 19, p. 095001, sep 2017.

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UIB Universitat de les Illes Balears