

Confined Active Matter

Aggregation and Segregation of Confined Active Particles

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Dynamics of Self-Propelled Particles Under Strong Confinement

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Recommended with a commentary by Charles Reichhardt and Cynthia Reichhardt, Los Alamos National Laboratory

When a gas of particles is placed in a confined environment such as a room or box, the particles can bounce off the wall creating a pressure. In fact, the system can readily be very well described by the ideal gas law $PV = nRT$, where P is the pressure, V is the volume, and T is the temperature. This means that if one increases the temperature while holding the volume fixed, the pressure will increase due to the increased energy the particles have when they strike the walls and the increased rate at which the particles strike the walls. Additionally, if the volume is fixed, the shape of the container has no effect on the pressure. One picture of an ideal gas is randomly walking particles that explore all space in the container with equal probability. As the temperature increases, the particles diffuse faster. Since the diffusion constant obeys the Einstein relation $D = \mu k_b T$, the faster the particles can diffuse, the higher the pressure. Additionally, if one places all particles in one corner of the container as an initial state, the particles rapidly diffuse throughout the whole system, filling it evenly. If a second species of gas particles is added to the system then the pressure again should increase and the two gas species will become evenly mixed.

All this can change if the particles are not thermal but are active or self-driven. Active systems include swimming bacteria that undergo run-and-tumble dynamics and self-motile colloids that perform driven Brownian motion [1,2]. The root mean square displacement of a single active particle shows superdiffusive or ballistic behavior at shorter times since the particles are effectively ballistically moving in a fixed direction, while at long times the particles exhibit diffusive behavior [3]. By increasing the mobility or swimming speed of the particles, the long-time effective diffusive constant increases as would be expected. At first glance it may seem that active system might not have that many qualitative differences from confined thermal particles. For example, just by increasing the run speed of the active particles, the pressure they exert on the walls of a container should naturally increase. If the active particles are initially placed in one corner of the container they should spread evenly throughout the container over time. In fact one could think that the run speed is simply proportional to an effective temperature, such that if the particle moves faster or has an increased running length, this should be like increasing the temperature, making it possible to construct an active matter gas law with $PV \propto$ mobility.

It turns out that active matter particles in confinement instead exhibit very different behaviors than that of thermal particles in confinement. Recently, Fily *et al.* (arXiv:1402.5583) considered a remarkably simple system of non-interacting self-propelled particles confined in a box and studied the effect of changing the box geometry. When at least one dimension of the box is smaller than the persistence length of the active particles, the authors find that the shape of the box has an effect on the spatial distribution of the particles. For example, for a 2D ellipse there is a high density of particles in regions with stronger curvature, while at sharp corners there can be a very high density of particles. This

means that the pressure exerted by the active matter is not uniform on the walls, and that simply by changing the geometry, the particle distribution in the system can be modified. Figure 1(a) shows a schematic of how purely Brownian particles, which fill space uniformly, would behave in a confined geometry near a corner, while Fig. 1(b) shows what would happen for active matter particles with a persistence length longer than the container side, where the particles concentrate in the corners.

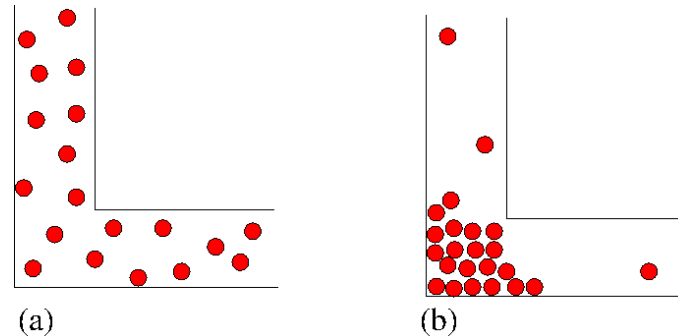


Figure 1: (a) Brownian particles (black dots) in a confined geometry with a corner, where the particles fill space uniformly. (b) Active particles with a persistence length of the motion that is larger than the container width. The particle accumulate in the corners.

The accumulation of active or self-driven particles in certain regions occurs since when a particle strikes a wall it does not bounce off the wall but keeps trying to move in the same direction, pressing against the wall. After some time the swimming direction of the particle changes due either to a tumbling event or to a gradual reorientation and the particle can move away from the wall. The longer the persistence time of the particles, the longer an individual particle will spend pushing against a wall. Particles that strike a wall at an angle rather than head-on can slide along the wall until encountering a corner, where they become trapped. The sharper the corner or the higher the local curvature, the longer the particles can remain trapped. Such trapping effects for active particles have already been observed in experiments [2] and simulations [4,5,6,7] of bacteria skimming along walls in the presence of sharp corners. This effect could have a variety of applications for the sorting of active matter particles. For example, for an active matter particle carrying cargo, by placing high curvature or corners at target areas for cargo delivery it is possible to effectively deliver more cargo to these areas. Additionally, this effect could also give insight into how certain spatial distributions of bacteria arise in nature. When bacteria become sufficiently dense, they can sometimes form a plaque or biofilm. If corners are places in which swimming bacteria naturally accumulate, they could serve as nucleation sites for the initiation of biofilm growth. Understanding bacterial biofilm growth could have a variety of applications in pharmaceutical and medical fields.

One might think that such corner-concentrating behavior arises in active matter systems only in the limit of non-interacting particles, but that once interactions between the particles are included the system would effectively "thermalize." It turns out, however, that when interactions are introduced, not only do the curvature effects persist, but new types of phenomena arise. Yang *et al.* (arXiv:1403.0697) considered interacting active matter particles confined in a box. Again, for the case of an ideal gas the particles would fill space evenly as shown schematically in Fig. 2(a); however, when the particles are active the authors find that they form clusters on the sides of the walls leaving a gap in the center as illustrated in Fig. 2(b). If the active particles have a size distribution, size segregation can occur in which one species of particles is closer to the wall than the other species. Since active systems are ubiquitous in biological systems such as crawling cells, one can ask how different types of cells segregate to form specialized tissues. The work of Yang *et al.* suggests that such behavior may arise simply due to the combination of confinement with activity. Yang *et al.* also showed that the pressure

on the walls in the active matter system exhibits significant deviations from the ideal gas law and that it is even possible for the pressure to decrease with increasing particle density. Another recent study by Mallory *et al.* [8] on confined active matter also indicated that the pressure deviates strongly from the ideal gas law.

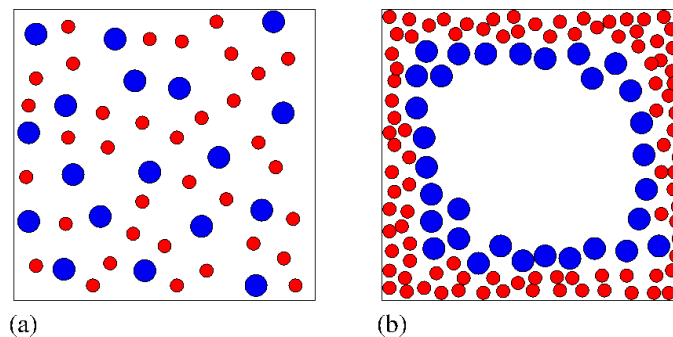


Figure 2: (a) Two species of Brownian particles in a box mix and fill the space uniformly. (b) Two species of active particles where the persistence length is larger than the box cluster along the walls and even exhibit phase segregation.

These papers combined with other recent results show that even the simplest active matter system can exhibit remarkably different behaviors than that observed for thermal systems, indicating that active matter systems can really be considered as a new type or state of matter. The ability to understand how active matter particles can accumulate on walls or at sharp corners could also have a wealth of applications in controlling microorganism accumulations in natural and man-made structures and could usher in a new type of dynamical self assembly.

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