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Active Matter on Asymmetric Substrates

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ABSTRACT

For collections of particles in a thermal bath interacting with an asymmetric substrate, it is possible for a ratchet effect to occur where the particles undergo a net dc motion in response to an ac forcing. Ratchet effects have been demonstrated in a variety of systems including colloids as well as magnetic vortices in type-II superconductors. Here we examine the case of active matter or self-driven particles interacting with asymmetric substrates. Active matter systems include self-motile colloidal particles undergoing catalysis, swimming bacteria, artificial swimmers, crawling cells, and motor proteins. We show that a ratchet effect can arise in this type of system even in the absence of ac forcing. The directed motion occurs for certain particle-substrate interaction rules and its magnitude depends on the amount of time the particles spend swimming in one direction before turning and swimming in a new direction. For strictly Brownian particles there is no ratchet effect. If the particles reflect off the barriers or scatter from the barriers according to Snell's law there is no ratchet effect; however, if the particles can align with the barriers or move along the barriers, directed motion arises. We also find that under certain motion rules, particles accumulate along the walls of the container in agreement with experiment. We also examine pattern formation for synchronized particle motion. We discuss possible applications of this system for self-assembly, extracting work, and sorting as well as future directions such as considering collective interactions and flocking models.

Keywords: Colloid, optical traps, active matter

1. INTRODUCTION

There have been a number of experiments examining the behavior of colloids interacting with ordered substrates such as two-dimensional square and triangular trap arrays created by optical means.[1-8] Many of the observed orderings for repulsively interacting colloids on periodic substrates have similar structures to those of vortices in type-II superconductors with periodic arrays of pinning sites.[9-12] The colloids and vortices can be driven over the substrates via an applied current, fluid flow, electric fields, or other optical means.[13-22] It is also possible to create systems with asymmetric substrates which produce directed motion of particles even in the absence of an external dc drive.[23,24] By applying an ac drive or by flashing the substrate, a net dc flow of particles can be induced which is termed a ratchet effect.[25] In two dimensions ratchet effects can occur in the presence of symmetric substrates when some other symmetry is broken, such as with a rotating ac drive[26-28] or by dynamically switching the substrate in a certain order.[29-31] The ratchet effect has been demonstrated for colloids on asymmetric substrates[23,24] and symmetric substrates with asymmetric drives,[28,31] for cold atom systems with flashing substrates,[32,33] for vortices in type-II superconductors with asymmetric pinning sites,[34-38] for vibrated granular matter on asymmetric substrates,[39,40] and for driven liquid drops on asymmetric heated plates.[41] Applications of the ratchet effect include sorting of different particles which ratchet at different rates over the substrate. In the overdamped single particle limit the ratchet effect generally occurs in a single direction; however, in collections of interacting particles, ratchet reversals can arise where the dc flow reverses as a parameter is varied.[37,38,40,42]

In all the ratchet systems mentioned above there is some form of external drive, such as a single ac drive, flashing of the substrate, or multiple external oscillating drives. There are many systems, termed active matter systems, that exhibit motion in the absence of any external drive. Examples include self-catalyzing colloidal particles,[43] microscopic artificial swimmers,[44] swimming bacteria, and active cells.[45] Recently, experiments were conducted for swimming bacteria in the presence of an array of asymmetric funnels.[46] No directed motion occurs

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for Brownian particles or nonswimming bacteria, but when swimming bacteria are added, a ratchet effect occurs and the bacteria concentrate on one side of the funnel array. Due to the complexity of the bacterial system, there are a wide variety of possible mechanisms for the concentration including hydrodynamic interactions, chemotaxis, or collective motions of the bacteria; however, a simple model of individual particles undergoing run and tumble dynamics along with a wall-following rule reproduces all of the experimental observations including the buildup of particles in the funnel tips and along the walls.[47] In this model, the particles move in a single direction over a run length l_r during a fixed run time τ_r, which is the time between tumbling events. Every τ_r simulation time steps, the particles randomly reorient and move in a new single direction over a distance l_r until the next tumbling event a time τ_r later. When the particle encounters a barrier, it moves along the barrier with a speed determined by the component of its running motion that is parallel to the barrier until the next tumbling event or until reaching the end of the barrier. If τ_r is small, l_r is small and the particles act more Brownian-like, with no rectification occurring for the limit of infinitesimal τ_r. The addition of steric interactions or thermal fluctuations reduces the rectification, while the rectification is enhanced when l_r is increased. With a similar model it was numerically shown and demonstrated in experiment that an asymmetric fly-wheel rotates in a preferred direction in the presence of a bacterial bath.[48-50] Other experiments have also shown directed cellular motion over asymmetric substrates[51-53] and even different directions of motion for different cell types on the same substrate.[54] Unlike the bacterial case, the mechanics of how the eukaryotic cells move is very important and the latter cannot be modeled simply by point particles. These studies open a new field of controlling active matter using periodic and asymmetric substrates. If the motion of self driven particles can be well controlled, it may be possible to use the particles to perform microscopic work such as transporting larger obstacles or cargo. Additionally, biological sorting could be achieved via ratchet effects. In this work we investigate the rules for run-and-tumble particles which generate a net dc motion of active matter in the presence of asymmetric barriers. We find that if the particles are fully aligned with the barriers, a much stronger rectification effect occurs. If the particles reflect or scatter off the barriers than no ratchet effect occurs even for very large l_r. This shows that the rectification requires the breaking of detailed balance in the interactions with the asymmetric barriers. We also find that there is a build up of particles along the barriers similar to what is observed in experiment.[47] This build up is due to the wall following rule combined with the finite size of the system. If the tumbling times of the particles are synchronized, we find that patterned moving density fronts of particles occur after the particles accumulate in corners of the containers or in the funnel tips.

2. COMPUTATIONAL MODEL

Figure 1 shows an image of our system which consists of an $L \times L$ two-dimensional box of length $L = 99$ with confining walls in the x and y directions containing N_a active particles. In the center of the system is an array of asymmetric funnels, placed in the same geometry used in the experiments for the swimming bacteria.[46] The particle density is $\rho = N_a/L^2$. The particles move in an overdamped media without hydrodynamic interactions according to the overdamped equation of motion

$$\eta \frac{d\mathbf{R}_i}{dt} = \mathbf{F}_i^m(t) + \mathbf{F}_i^B + \mathbf{F}_i^{pp} + \mathbf{F}_i^T. \tag{1}$$

Here $\eta = 1$ is a phenomenological damping term. The time dependent motor force $\mathbf{F}_i^m(t)$ is represented by run and tumble dynamics. Here $|\mathbf{F}^m| = 2.0$ while $\hat{\mathbf{F}}_i^m$ is selected randomly and changed every τ_r simulation time steps. The resulting run length $l_r = \tau_r \delta t |\mathbf{F}^m|$ where $\delta t = 0.005$ is the simulation time step size. Fig. 2(a) shows a single active particle with $\tau_r = 1000$ and $l_r = 10$ moving in straight paths for extended distances before randomly orienting and moving in other directions, producing a time average velocity of zero. With smaller τ_r the length scale over which the motion appears Brownian decreases, as shown in Fig. 2(b) for $l_r = 1.0$. Many active matter systems contain thermal fluctuations which we represent as Langevin kicks with the term $\mathbf{F}_i^T$, where $\langle F_i^T \rangle = 0$ and $\langle F_i^T(t)F_j^T(t') \rangle = 2\eta k_B T \delta_{ij}\delta(t-t')$ where k_B is the Boltzmann constant. Fig. 2(c) illustrates the combination of run and tumble dynamics with thermal fluctuations. We initially consider $F^T = 0.0$ since in many active matter systems at room temperature, such as bacteria, the thermal fluctuations are small on the scale of the particles. The term $\mathbf{F}_i^{pp}$ is the particle-particle interaction force which is modeled as simple short ranged steric repulsion. The term $\mathbf{F}_i^B$ is the force from the barriers which are each modeled by two half-parabolic domes of
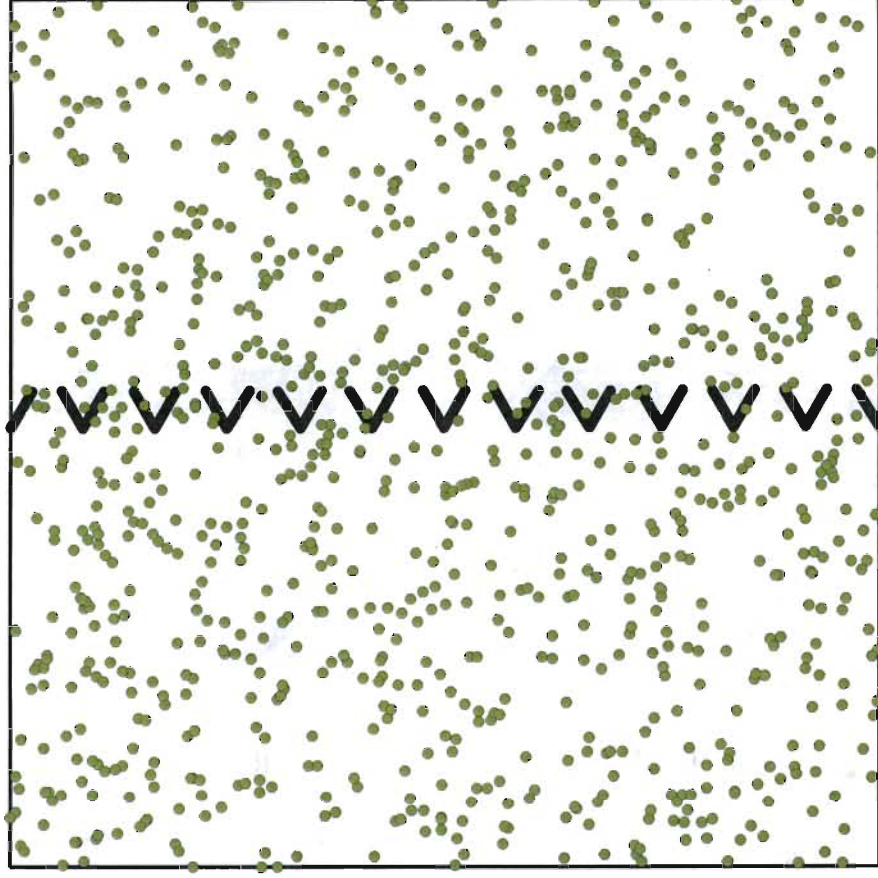
Figure 1. A snapshot of the system which consists of a confining box with an array of asymmetric barriers (heavy lines) and N_a active particles (green dots) that obey different rules for motion and interactions with the walls and barriers.

strength $F_B = 30$ and radius of $r_B = 0.05$ which repel particles along the direction perpendicular to the trap axis.

$$\mathbf{F^B}_i = \sum_{k=0}^{N_B} \frac{F_B r_1}{r_B} \Theta(r_1) \hat{\mathbf{R}}_{ik}^{\pm} + \frac{F_B r_2}{r_B} \Theta(r_2) \hat{\mathbf{R}}_{ik}^{\perp}. \tag{2}$$

Here the total number of barriers including the confining walls is $N_B = 28$, $r_1 = r_B - R_{ik}^{\pm}$, $r_2 = r_B - R_{ik}^{\perp}$, $R_{ik}^{\pm} = |\mathbf{R}_i - \mathbf{R}_k^B \pm L_B \hat{\mathbf{p}}_{||}^k|$, $\hat{\mathbf{R}}_{ik}^{\pm} = (\mathbf{R}_i - \mathbf{R}_k^B \pm L_B \hat{\mathbf{p}}_{||}^k)/R_{ik}^{\pm}$, $R_{ik}^{\perp} = |(\mathbf{R}_i - \mathbf{R}_k^B) \cdot \hat{\mathbf{p}}_{\perp}^k|$, $\hat{\mathbf{R}}_{ik}^{\perp} = [(\mathbf{R}_i - \mathbf{R}_k^B) \cdot \hat{\mathbf{p}}_{\perp}^k]/R_{ik}^{\perp}$. $\mathbf{R}_i(\mathbf{R}_k^B)$ is the position of particle i (barrier k), and $\hat{\mathbf{p}}_{||}^k$ ($\hat{\mathbf{p}}_{\perp}^k$) is a unit vector parallel (perpendicular) to the axis of barrier k. The funnels are modeled as two barriers meeting at a common end point at angles θ and $\pi - \theta$ with the x-axis and the tips of adjacent funnels are spaced a distance 8.25 apart along the x direction.

3. RULES PRODUCING RECTIFICATION FOR NON-INTERACTING PARTICLES

We first consider the case of no thermal fluctuations and no steric interactions between particles. In previous work, a particle encountering a barrier had the component of its motion perpendicular to the barrier canceled but experienced no reorientation of $\mathbf{F}_i^m$ by the barrier.[47] This behavior, termed Rule I, is is illustrated in the schematic in Fig. 3(a). Here we consider three additional barrier interactions. In Rule II, $\mathbf{F}_i^m$ is realigned to be parallel with the barrier. This is a realistic assumption for many types of active matter such as elongated
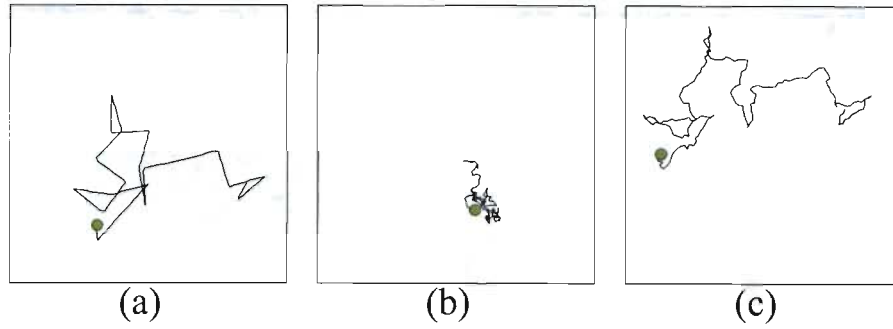
Figure 2. The trajectories of a single active particle undergoing run and tumble dynamics. (a) $l_r = 10$. (b) $l_r = 1$. (c) The same as in (a) but with an added thermal noise component with $F^T = 10.0$.
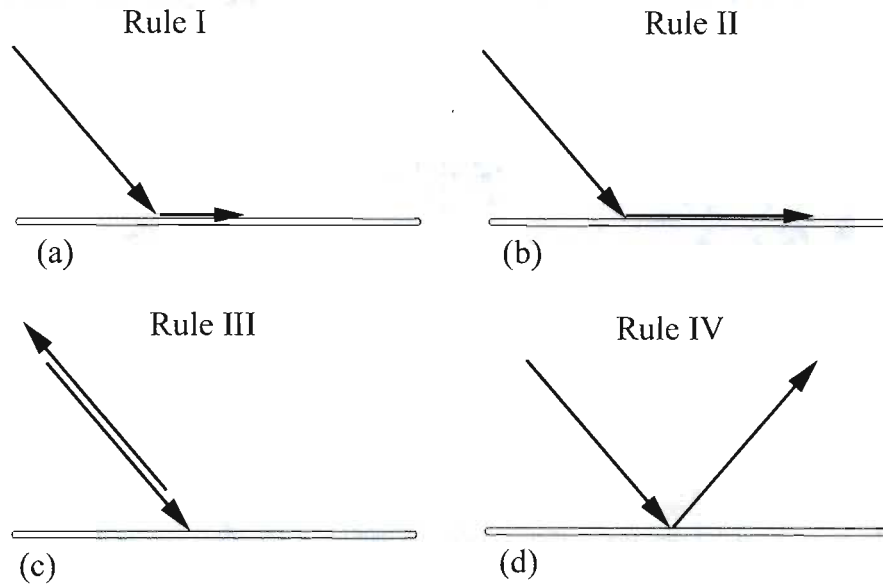

Figure 3. Different rules for the particle-barrier interactions. (a) Rule I. The particles move with the component of $\mathbf{F}_i^m$ that is parallel to the barrier. (b) Rule II. $\mathbf{F}_i^m$ is realigned to be completely parallel to the barrier. (c) Rule III. The particles reflect off the barriers. (d) Rule IV. The particles scatter off the barriers.

bacteria, which can align their swimming with a wall due to hydrodynamic interactions. In Rule III, $\mathbf{F}_i^m$ is reversed so that the particles reflect back into the direction from which they came, as shown in Fig. 3(c), while in Rule IV, $\mathbf{F}_i^m$ is reflected across a line perpendicular to the barrier so that the particles scatter off the barrier, as illustrated in Fig. 3(d).

We now consider Rule I, partial alignment with the barriers, for short and long l_r as illustrated in Fig. 4. For $l_r = 0.01$ after 100 tumbling events in Fig. 4(a), there is no rectification and the density $\rho^{(1)}/\rho$ in the upper channel equals the density $\rho^{(2)}/\rho$ in the lower channel, as shown in Fig. 5. For $l_r = 180$, there is a buildup of particles in the upper chamber as shown in Fig. 4(b), and the dependence of $\rho^{(1)}/\rho$ and $\rho^{(2)}/\rho$ on time has a shape very similar to the form found in experiments,[46] as illustrated in Fig. 5. The rectification mechanism for long l_r is illustrated in Fig. 6. When a particle approaches a funnel from below, it is guided along the barrier and moves into the upper chamber as long as τ_r is long enough that it does not change direction before reaching the upper chamber. On the other hand, when a particle approaches a funnel from above, it is guided into the closed
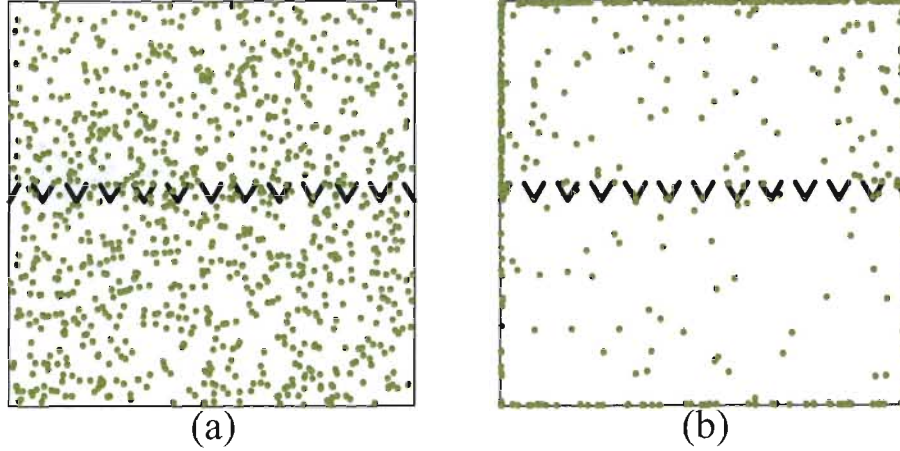
Figure 4. Image of the sample after 100 tumbling events for Rule I. (a) At $l_r = 0.01$, the particle density is equal on both sides of the chamber. (b) At $l_r = 180$ the particle density has substantially increased in the upper chamber with particles accumulating along the walls and in the funnel tips.

tip of the funnel where it remains trapped until a new tumbling event sends it back into the upper chamber. For small l_r the same barrier interaction rules still apply; however, due to the short time between tumbling events, the particle spends so little time moving along the barrier that its motion cannot be guided and no rectification occurs. This result shows that it is the combination of the long running time and the breaking of detailed balance in the particle-barrier interactions that lead to the rectification. Fig. 7 shows a plot of $r = \rho^{(1)}/\rho^{(2)}$ versus l_r for the Rule I sample. The amount of rectification increases with increasing l_r. In the limit of small l_r where the interactions between the particles and the barriers are in the Brownian limit there is no rectification.

When we employ Rule III or Rule IV we find no rectification, as shown in Fig. 8 where we plot r for the four different rules in a sample with $l_b = 300$. Regardless of the value of l_r, Rules III and IV do not produce rectification of the particles due to the fact that they preserve detailed balance for the interactions of the particles with the barriers, which is enough to prevent rectification.

We note that the amount of rectification varies with other system parameters such as the angle of the funnels, the overall size of the funnels relative to l_b, and the spacing between adjacent funnels. In general, if the funnels are made larger for fixed l_r the rectification is reduced, since this has the same effect as holding the funnel size constant and reducing l_r. Increasing the spacing between the funnels reduces the effect since there is simply more space for particles to freely pass from the upper chamber to the lower chamber, producing a larger amount of backflow and lowering the efficiency of the ratchet. As a function of the angle between the funnel arms, the ratchet effect is generally optimized near 50 to 60 degrees.[47]

4. STERIC AND THERMAL INTERACTIONS

We next consider the effect of adding a short range steric repulsion between the particles which is modeled as a stiff spring of finite radius which produces a force

$$\mathbf{F}_i^S = \sum_{i \neq j}^{N_a} \frac{f_a r_3}{r_s} \Theta(r_3) \hat{\mathbf{R}}_{ij} \tag{3}$$

Here $r_3 = r_a - R_{ij}$, $R_{ij} = |\mathbf{R}_i - \mathbf{R}_j|$, $\hat{\mathbf{R}}_{ij} = (\mathbf{R}_i - \mathbf{R}_j)/R_{ij}$, and $f_a = 150$ is the force coefficient.

In Fig. 9(a) we plot r vs ρ for a system with $l_r = 20$ and steric interactions under Rule I. Here the rectification decreases with increasing density. The interacting particles interfere with each other's motion in several ways. Particles that strike the barriers at an angle that is nearly perpendicular to the barrier move very slowly along
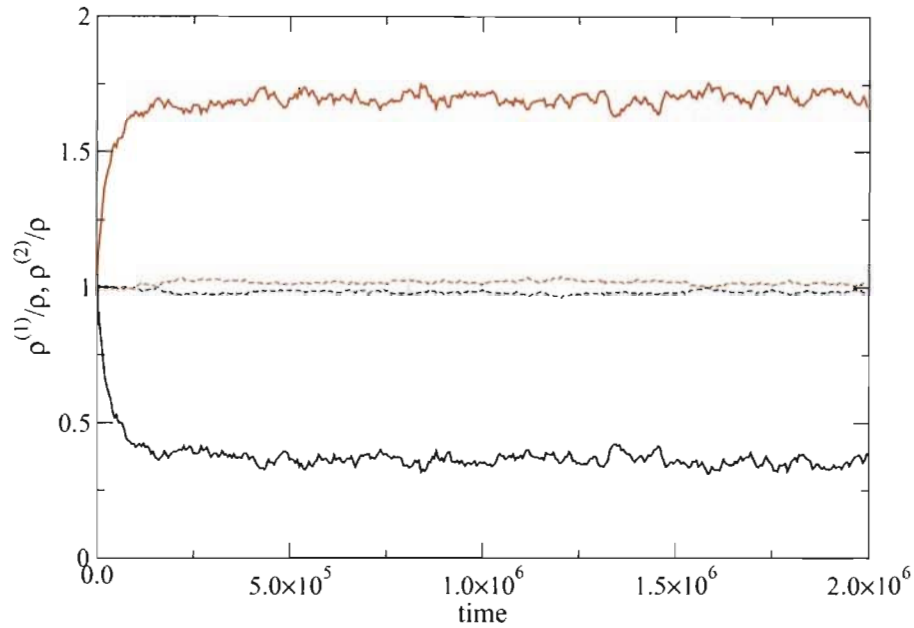
Figure 5. $\rho^{(1)}/\rho$ and $\rho^{(2)}/\rho$ vs time in simulation time steps for the system in Fig. 4 under Rule I. Dotted lines: $l_r = 0.01$ from Fig. 4(a) where the density is almost the same in each chamber. Upper heavy line: $\rho^{(1)}/\rho$ for the $l_r = 180$ system from Fig. 4(b); lower heavy line: $\rho^{(2)}/\rho$ for the system from Fig. 4(b).
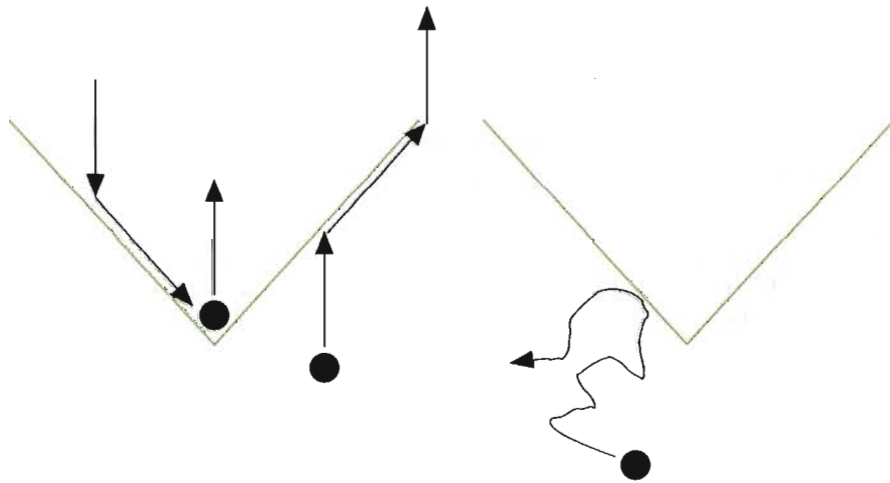

Figure 6. A schematic of the rectification mechanism under Rule I and Rule II. Left panel: A particle approaching the funnel from above aligns with the barrier and moves into the funnel tip where it is trapped. After the next tumbling event the particle may escape from the funnel tip and move back into the upper chamber. A particle approaching the funnel from below aligns with the barrier and is guided into the upper chamber. Right panel: For very short l_r, the particle spends little to no time interacting with the barrier and its motion cannot be guided by the spatial asymmetry of the barrier.
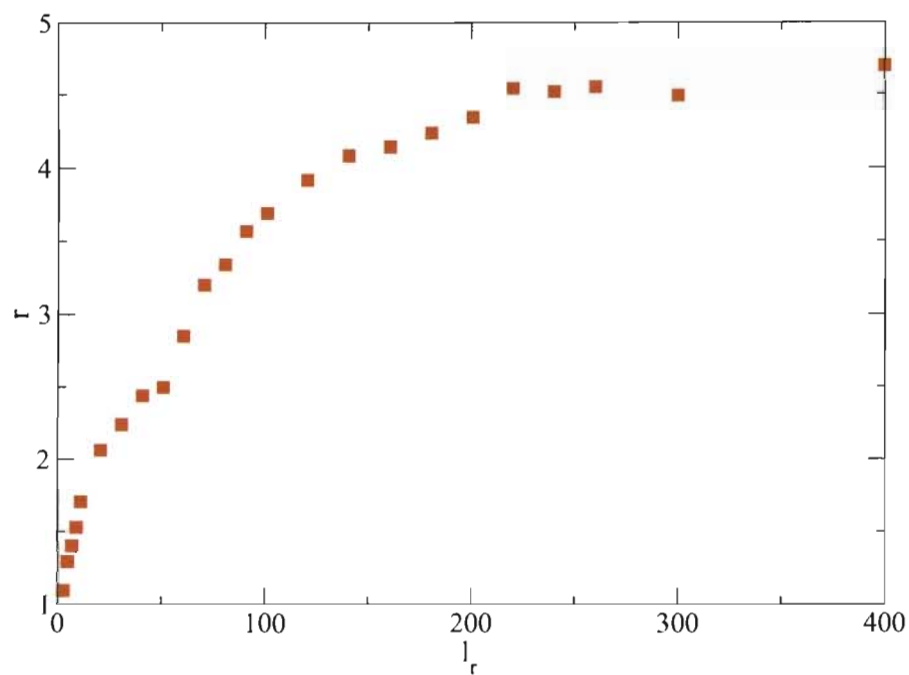
Figure 7. The ratio of the particle densities $r = \rho^{(1)}/\rho^{(2)}$ vs l_r for the system with Rule I. For small l_r the rectification is lost.
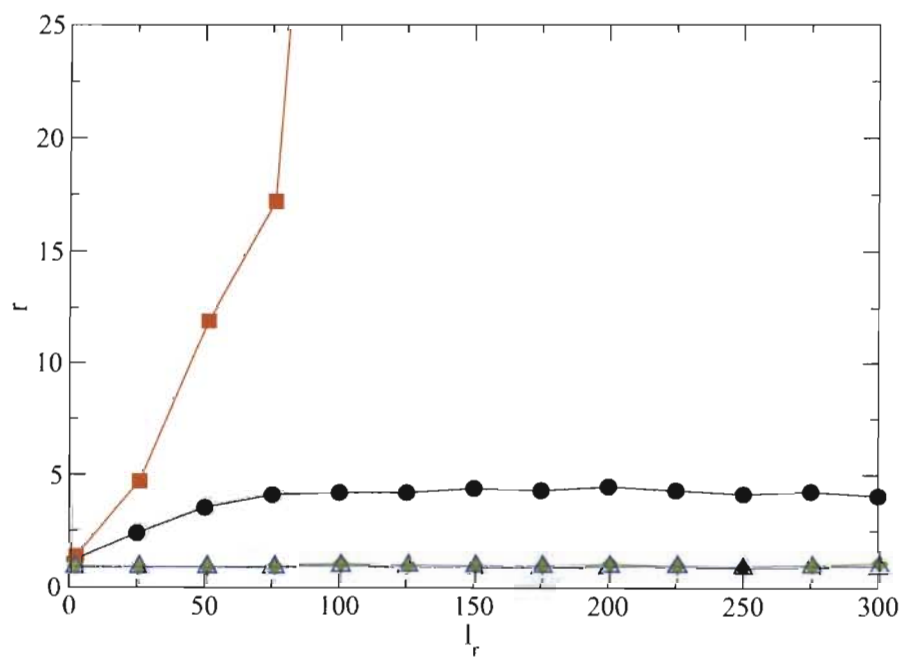

Figure 8. The value of r after 6000 tumbling events for a system with $l_r = 300$ for Rule I (filled circles), Rule II (filled squares), Rule III (filled diamonds), and Rule IV (open triangles). Here only Rules I and II produce rectification.
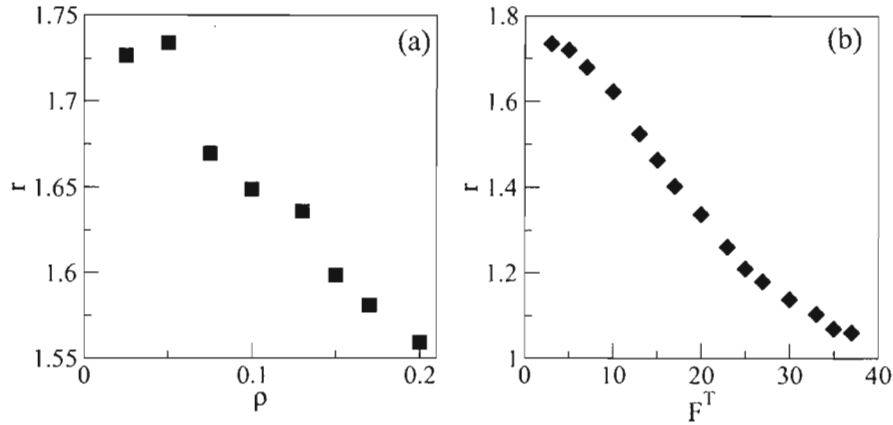
Figure 9. (a) r vs ρ for a system with steric interactions under Rule I at $l_r = 20$. Here r decreases with increasing ρ. (b) r vs the thermal force F^T for a system with no steric interactions under Rule I at $l_r = 20$. The rectification is reduced as the magnitude of the thermal fluctuations increases.

the barrier. These particles get in the way of other particles that strike the barrier at lower angles and that would otherwise move relatively quickly along the barrier. This interaction decreases the efficiency of the ratchet. The buildup of particles along the walls also becomes much more apparent for the sterically interacting particles, as illustrated in Fig. 10. A similar formation of excess density along the walls occurred in the experiments of Ref.[46,55] In Fig. 9(b) we illustrate the effects of adding thermal noise to a system of particles without steric interactions under Rule I with $l_r = 20$. The plot of r versus F^T shows that the rectification is strongly reduced as the thermal fluctuations begin to dominate the motion of the particles and the system enters the Brownian limit.

5. SYNCHRONIZED SWITCHING AND PATTERN FORMATION

Up to this point we have considered the effects of random tumbling events. All of the particles had equal τ_r; however, at the beginning of the simulation each particle was assigned a randomly chosen amount of time $0 < t < \tau_r$ after which the first tumbling event for that particle would occur. This desynchronized the switching of the particles. It could, however, be possible for certain systems to have synchronized tumbling events for all particles. For example, this would occur if a periodically applied external field activated the tumbling, so that all of the particles would change direction simultaneously. For open systems or samples with periodic boundary conditions, pattern formation would not be expected to occur; however, in the confined box and funnel geometry that we study we find that pattern formation in the form of expanding fronts of particles occurs when the switching events are synchronized for particles that have no steric interactions. In Fig. 10(a,b) we illustrate the formation of moving fronts of particles in a system with no steric interactions at $l_r = 80$ under Rule I with synchronized tumbling times. Density fronts are emitted by the four corners of the container and to a lesser extent also from the ends of the funnels. These fronts move out in a growing circular pattern, decreasing in density as they spread until the structures break up due to interactions with the walls. The pattern forms since the particles can effectively collapse into the corners and the funnel tips due to their lack of steric interactions; the particles are trapped in these locations due to the barrier interaction Rule I. If τ_r is long enough essentially all the particles will become trapped in the corners and funnel tips. Since the tumbling events are synchronized, the particles move out from each trapping point in a circular pattern after a switching event. In our system we observe only a semicircle of motion due to the confinement by the walls. The fronts are clearly defined only for sufficiently large τ_r since for short τ_r the particles do not have enough time to become highly concentrated in the corners and funnel tips. This type of pattern formation is strongly reduced for particles with steric interactions since the interactions reduce the ability of the particles to become concentrated at a point; however, some remnant of the moving fronts still can be observed when steric interactions are present.
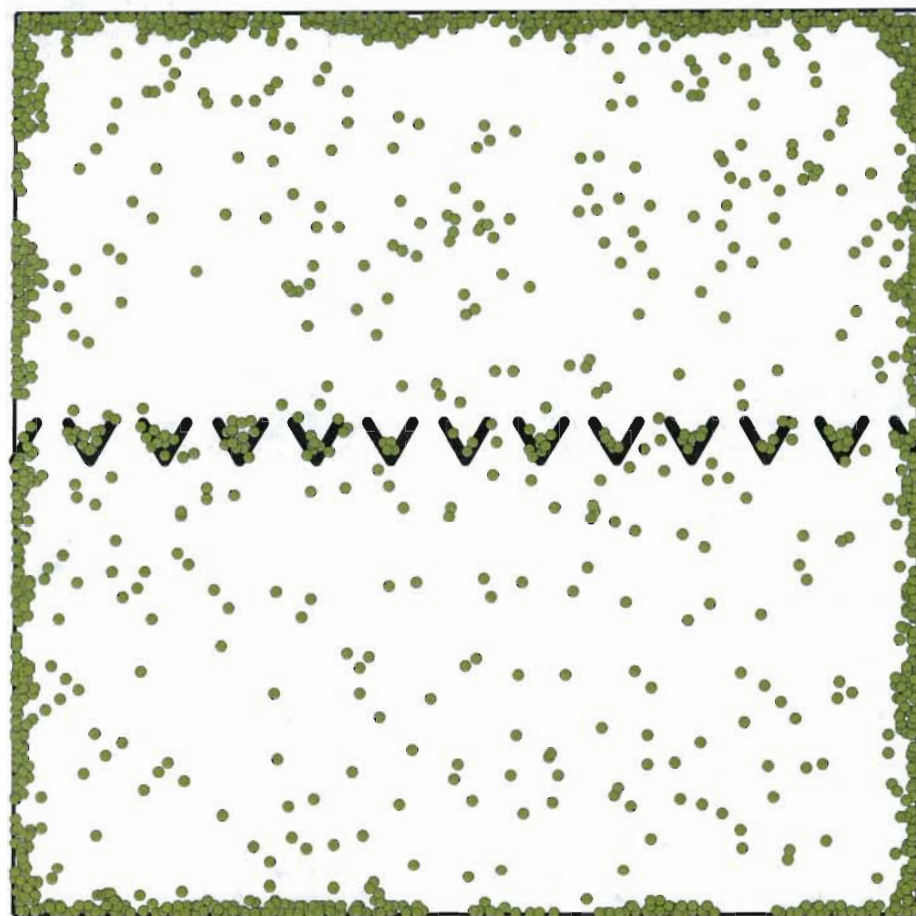
Figure 10. The build up of particles along the walls and inside the funnels for a system with Rule I and sterically interacting particles at $l_r = 120$. This same effect is observed in experiments.
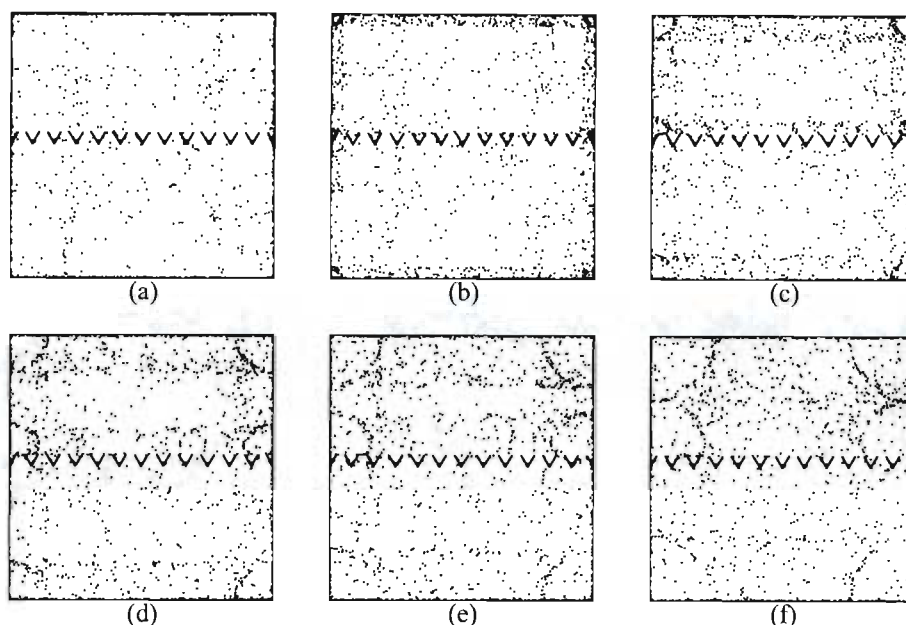
Figure 11. The formation of moving particle fronts for a system with Rule I, no steric interactions, $l_r = 80$, and synchronized tumbling times, shown as consecutive snapshots of the system taken at equal time intervals. The particles accumulate in the corners of the container and are released as a semicircular density wave after each switching event.

6. DISCUSSION AND FUTURE DIRECTIONS

This work in conjunction with experiments shows that simple substrates can be used to create directed motion in self-driven particle systems. This opens the possibility for an entirely new class of ratchets based on microscale systems which could be used for sorting different species of active particles, guiding particles to move in certain directions, and possibly even extracting work out of such systems. Our results show that thermal fluctuations can strongly reduce the efficiency of the directed motion. For large colloids and many biological systems, thermal effects are generally small on the scale of the particles; however, if nanoscale self-driven particles are considered then thermal effects will be relevant. Our work and other models of this type of system include only point particles or elongated rods. It would be interesting to study ratcheting behavior for particles with more complicated shapes or for particles that contain internal degrees of freedom. For example, eukaryotic cells exhibit different types of mechanical mechanisms for locomotion such as pushing or pulling motions, and it could be possible to implement swimming rules that mimic such motions. We have studied only static substrates in our system; however, it should be possible to create dynamic substrates for self-driven particles similar to flashing ratchets, and such dynamic substrates might be much more effective in directing the motion of the particles. It would also be interesting to study different types of collective effects such as by introducing models for flocking or swarming behaviors or by adding longer range interactions between particles which could arise through hydrodynamic effects. Although the model we consider is mostly relevant for microscopic systems, similar effects could be tested for larger scale systems such as individual or collectively moving insects, animals, and birds. Another possibility would be to study self-driven particles that have an intrinsic asymmetry as they move through symmetric or asymmetric substrates.

7. SUMMARY

We have shown that a new type of ratchet system can arise in systems of self-driven particles or active particles in asymmetric geometries. Unlike most ratchet systems where some form of external ac force or flashing potential is required to induce a ratchet effect, the self-driven particle system can exhibit a ratchet effect in the absence

of external forcing. In our system we consider active particles that move with a run-and-tumble dynamics of the type found in bacterial systems where the particles move in a single direction for a fixed time before undergoing a tumbling event, randomly reorienting, and then moving for a fixed period of time in a new direction. We studied different rules for the interactions between the particles and the barriers, including alignment or partial alignment with the barrier which causes the particles to follow the barriers as well as reflection and scattering interactions. When the particles are allowed to move along the barriers and when the time between tumbling events is sufficiently long, we observe rectification of the particles by the barriers. We also find a buildup of particles along the walls and inside the funnel tips. Both the rectification and the buildup of the particles along the barriers are in excellent agreement with experimental observations. Under these same wall interaction rules, if the time between tumbling events is very small the motion of the particles becomes more Brownian-like on the length scale of the barriers and the rectification is lost. For reflection and scattering of the particles off the barriers the rectification is lost even for very long times between tumbling events. These results show that it is the combination of the running length and the breaking of detailed balance in the particle-barrier interactions that produce the rectification. We have also found that if the tumbling times for the particles are synchronized, pattern formation occurs in the form of moving density fronts generated after each switching event due to the concentration of particles in the corners and funnel tips. The addition of thermal effects or steric interactions generally reduces the effectiveness of the rectification. Future directions to pursue include more complicated shapes and interactions for the individual particles as well as the addition of collective effects.

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