Collective and emergent dynamics in active systems

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Abstract: We study some non-equilibrium properties of active matter, such as self-propulsion, that causes the emergence of phenomena not observed in equilibrium systems. By applying the UCNA approximation we are able to derive a probability density function under stationary conditions that enables us to study the behaviour of active particles in the presence of a perturbation such as a hard wall modelled by a repulsive potential. From here, we calculate the adsorption near the wall and we study the dependence it has on activity. We find that adsorption grows approximately as the square root of the activity, regardless if the potential is strictly repulsive or repulsive and attractive in different regions of space.

I. INTRODUCTION

Self-propelled or active particles are particles that take energy from the environment an transform it into persistent motion. The study of self-propulsion is of wide interest because it is a characteristic that is found in many biological systems, for example, molecular motors or swimming bacteria. In recent years, extensive research has been carried out focusing on finding a model to properly describe the dynamics of active systems.

Brownian motion describes the motion of particles suspended in a fluid as a result of collisions with the fluid particles due to thermal agitation. Systems performing Brownian motion are in thermodynamic equilibrium. A characteristic of active systems, though, is the self-propulsion of its particles which drives the system far from equilibrium. Thus, Brownian motion fails to fully the motion of active systems. Among the most standard models which have emerged to describe active systems we find the active Brownian model and the Run-and-tumble model. In the active Brownian model, particles swim at fixed speed and their direction of motion changes gradually by angular diffusion. In the Run-and-tumble (RnT) model, which was first introduced to describe the motion of the *Escherichia coli* bacterium, particles move along straight paths with speed v (run) and after a certain time, called the persistence time, they experiment a random change in the direction of their motion (tumble), after which they continue to move in a straight line. Although these models are widely spread, they do not provide an analytic expression for the many-particle distribution function of the system.

The Gaussian coloured-noise is another model which describes the motion of active particles. Basically, it models the motion of a Brownian particle using the Langevin equation where a memory for the relaxation of the velocity is introduced. Thus, there are velocity correlations with time.

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An approximation to this model is the *Unified Colored Noise approximation* (UCNA). The relevance of UCNA is that, by eliminating the acceleration terms of the problem, it allows one to find an approximate probability distribution for many particles under stationary conditions called *Multidimensional unified coloured noise approximated stationary probability* (MUCNASP) and developed by Maggi, Marconi et al. in [4].

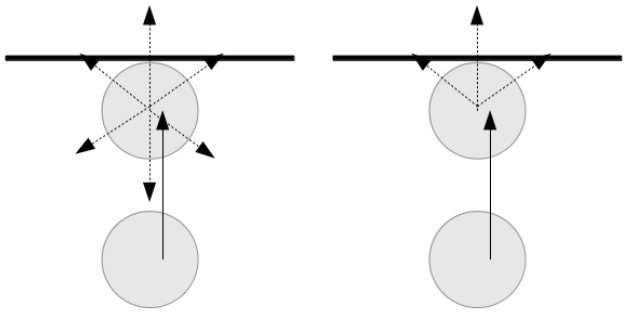

FIG. 1: Scheme of the effect of activity on the emergence of aggregation. Activity can be understood as the time correlations between the successive displacements that compose the random motion of a particle. If there are no correlations between successive displacements (left-hand figure) the system will not have a tendency to aggregate because the particle will have the same probability of staying attached to the wall as that of leaving it. However, if correlations exist it will take a certain amount of time for the particle to detach from the wall (right-hand figure) and so aggregation will appear. Full arrows: Direction of the first step. Dotted arrows: Possible directions of the next step.

The characteristic tendency of active particles to aggregate in the presence of an obstacle, despite there being no attractive inter-particles forces, can be the cause of different physical phenomena. Adsorption is a phenomenon by which gas, liquid or dissolved solid particles adhere to a certain surface. (Adhesion is the tendency for two different particles to cling to one another). A related phenomenon is wetting, which is the capacity of a liquid to be in contact with a solid surface without spreading

out.

In this project we study the aggregation of non-interacting active particles when subjected to a repulsive potential which models a hard wall. We also analyze the adsorption of particles to the hard wall and the influence that activity has in this phenomenon.

II. MODELLING A SYSTEM OF ACTIVE PARTICLES. THE UCNA APPROXIMATION.

We base our study on the theory exposed by Marconi et al. [1]. From the equations of motion of a system of Brownian particles with memory they derive the probability density function for one particle. We are going to work with this probability density function to study the motion of active particles subjected to a repulsive potential.

The Langevin equation describes a system of particles immersed in a fluid that undergo Brownian motion due to collisions induced by thermal agitation. Marconi et al. [1] introduce a memory associated to the relaxation of the velocity, modelled by a Gaussian coloured noise force, $\vec{v}_i$. The result is two coupled equations which fully describe the motion of active particles.

$$\dot{\vec{r}}_i = \frac{1}{\gamma}\vec{F}_i(\vec{r}_1, ..., \vec{r}_N) + D_t^{\frac{1}{2}}\vec{\xi}_i^t(t) + \vec{v}_i(t) \tag{1}$$

$$\dot{\vec{v}}_i(t) = -\frac{1}{\tau}\vec{v}_i(t) + \frac{D_a^{\frac{1}{2}}}{\tau}\vec{\eta}_i(t) \tag{2}$$

$\vec{F}_i(\vec{r}_1, ..., \vec{r}_N)$ is a conservative drag force proportional to the particles' velocity, $\dot{\vec{r}}_i$, and represents the friction done by the fluid. $\vec{\xi}$ simulates the thermal agitation of the fluid and is characterized by diffusivity, D_t. It is a white Gaussian noise vector, which means that it is a random vector that follows a Gaussian probability distribution and it is uncorrelated at different instants of time (Markovian), $\langle\vec{\xi}_i(t)\vec{\xi}_j(t')\rangle = 2\delta_{ij}\delta(t-t')$. $\vec{\eta}$ is also a white gaussian noise vector. $\vec{v}_i$ models self-propulsion, it is characterized by τ and D_a, and it is a coloured Gaussian noise vector. Therefore, it has a correlation over time that decays as $\langle\vec{v}_i(t)\vec{v}_j(t')\rangle = 2\frac{D_a}{\tau}\delta_{ij}exp(-|t-t'|/\tau)$, where τ is the correlation time. In the limit $\tau \to 0$ we go back to equilibrium and the vector will be uncorrelated at different instants of time.

The *Unified Colored Noise approximation* (UCNA) [7] introduces the condition of strong friction between the particles and the fluid. This allows us to drop the acceleration terms of the problem. The process is then assumed to have no memory. From Eq. (1) and applying the UCNA approximation we obtain

$$\dot{x}_i \simeq \sum_k \Gamma_{ik}^{-1}[\frac{1}{\gamma}F_k + D_a^{\frac{1}{2}}\eta_k(t) + D_t^{\frac{1}{2}}\xi_k^t(t)] \tag{3}$$

where the friction matrix is

$$\Gamma_{ik} = \delta_{ik} + \frac{\tau}{\gamma}\frac{\partial^2 U}{\partial x_i \partial x_k} \tag{4}$$

UCNA is valid for both small and large correlation times, τ, and for values of the friction strictly positive. Its accuracy improves for larger values of the friction.

By eliminating the fast degrees of freedom we obtain a Markovian process (without memory) out of the non-Markovian process we had at the beginning. It is important to mention, though, that we are still out of equilibrium and so there are still velocity correlations captured in the friction matrix, which now is not a constant but depends on the positions of particles.

According to Hänggi and Jung [7], the probability distribution function, $f_N(x_1, ..., x_N, t)$, of a process with no memory will evolve following a Focker-Planck equation,

$$\frac{\partial f_N(x_1, ..., x_N, t)}{\partial t} = -\sum_l \frac{\partial}{\partial x_l} J_l(x_1, ..., x_N, t) \tag{5}$$

In the case of vanishing probability currents, $J_l(x_1, ..., x_N, t) = 0$, Marconi et al. [1] obtain an expression for the stationary N-particle distribution function,

$$P_N(x_1, ..., x_N) = \frac{1}{Z_N}\exp\left(-\frac{H(x_1, ..., x_N)}{(D_a + D_t)\gamma}\right) \tag{6}$$

which is very similar to the Boltzmann distribution. We can identify $(D_t + D_a)\gamma$ with a temperature, T_s, which is the particle's energy due to diffusivity, taking into account that we are working with $k_B = 1$.

Applying the BGY hierarchy, Barrat et al. [5], enables us to trace out the dependence of the probability distribution on the positions of N-1 particles so that P_N only depends on the position of one particle, obtaining the equation for the single-particle density function. In the case we study there are no pairwise interactions between particles so the potential is due to the external field $u(x)$, which we choose to be a repulsive potential.

$$T_s\frac{d}{dx}\left(\frac{\rho^{(1)}(x)}{1 + \frac{\tau}{\gamma}u_{xx}(x)}\right) = -u_x(x)\rho^{(1)}(x) \tag{7}$$

where $u_x(x)$ and $u_{xx}(x)$ are the first and second derivatives of $u(x)$, respectively. Solving the differential equation,

$$\rho^{(1)}(x) = \rho_0\exp\left(-\frac{u(x) + \frac{\tau}{2\gamma}(u_x(s))^2}{T_s}\right)\left[1 + \frac{\tau}{\gamma}u_{xx}(x)\right] \tag{8}$$

This is the single particle probability density function in one dimension. ρ_0 is the probability density of the

volume and we have fixed its value to $\rho_0 = 1$. Considering $u(x) = u_0 f(x)$ we have rewritten the probabilty density,

$$\rho^{(1)}(x) = \rho_0 \exp\left(-\frac{u_0}{T_s}\left(f(x) + \frac{1}{2}Pe\frac{F_w}{F_a}(f_x(x))^2\right)\right)\left[1 + Pe\frac{F_w}{F_a}f_{xx}(x)\right] \tag{9}$$

We can identify three dimensionless parameters which determine the collective behaviour of the system. $\frac{u_0}{T_s}$ relates the energy of the wall to the diffusive energy of the particles. Consequently, the smaller $\frac{u_0}{T_s}$ is, the softer the wall is to particles. $\frac{F_w}{F_a} = \frac{u_0}{\gamma\sigma v_0}$ is the force that the wall exerts on the particles compared to the particles' force due to their velocity in a straight path, v_0. σ is the particles' size. $Pe = \frac{\tau v_0}{\sigma}$ is the Péclet number and compares the persistent distance (straight distance that a particle travels before reorienting its direction of motion) to the particles' size. This is the dimensionless parameter we use to measure the system's activity. It is important to notice that when there is no activity, that is Pe=0, the system is at equilibrium.

To quantify the amount of particles that aggregate in a region of space with respect to the particles in the volume we calculate the adsorption,

$$\Gamma = \int_0^\infty (\rho^{(1)}(x) - \rho_0)dx \tag{10}$$

III. RESULTS AND DISCUSSION

First of all we are going to show how the probability density is modified when the system is subject to different potentials. After that, we will discuss how the repulsive potential causes particles to aggregate and how the adsorption depends on the activity of the system.

A. Probability densities

We need to numerically compute the accumulation of particles when there is aggregation in the presence of a repulsive potential. To do so, we have developed a code implemented in Mathematica.

From the three parameters appearing in the density profile, Eq. 9, we choose to study the dependence of the adsorption with the Péclet because it is the parameter that measures the activity, as we mentioned before. We fix the other two parameters $\frac{u_0}{T_s} = \frac{F_w}{F_a} = 10$. Therefore, the energy of the wall is bigger than that of the particles and we ensure that the repulsive potential really models a hard wall which particles cannot penetrate.

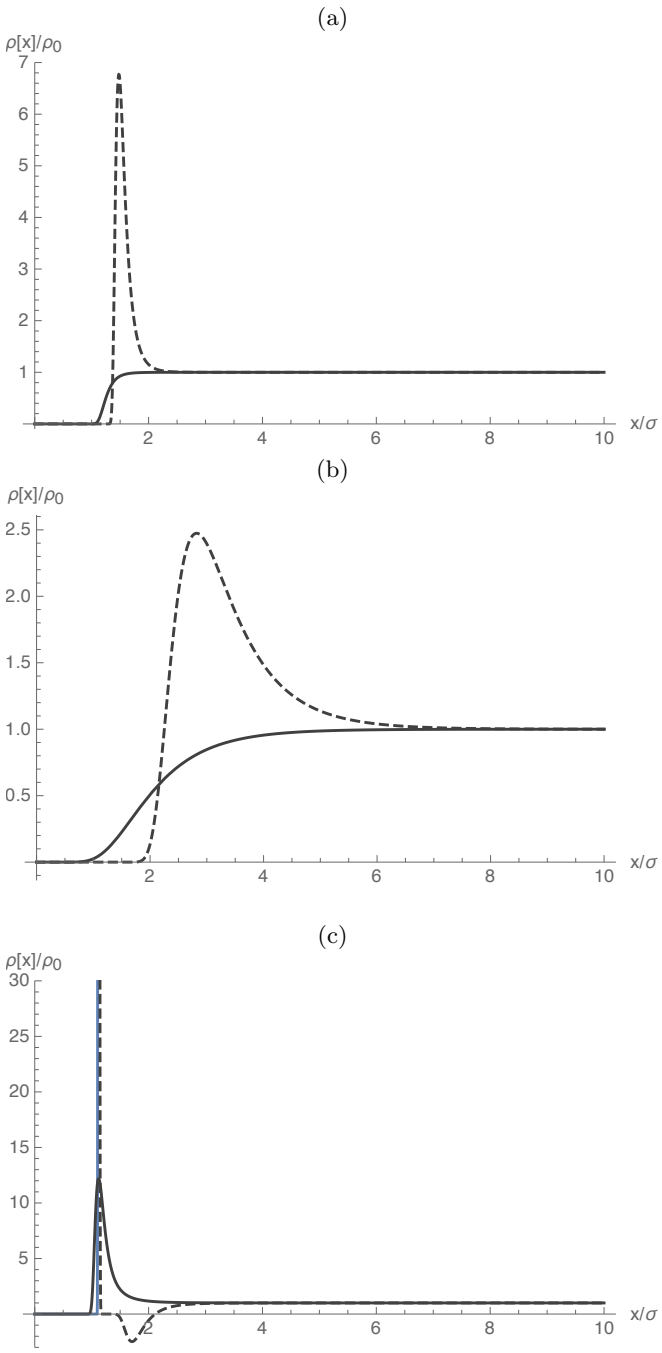

FIG. 2: Dashed lines: Density profiles for an activity value Pe=8 for potentials (a) $u(x) = u_0\frac{1}{x^{12}}$; (b) $u(x) = u_0\frac{e^{-x}}{x}$; (c) $u(x) = u_0(\frac{1}{x^{12}} - \frac{1}{x^6})$. Full lines: Density profiles at equilibrium for the same potentials.

To model the repulsive wall we use three different potentials. Two of them are completely repulsive, $u(x) = u_0\frac{1}{x^{12}}$ and $u(x) = u_0\frac{e^{-x}}{x}$, and the third one is the Lennard-Jones potential, which has both a repulsive and

an attractive region, $u(x) = u_0(\frac{1}{x^{12}} - \frac{1}{x^6})$.

In Fig. 2 above we show the probability densities for the three different potentials we have worked with. To plot the profile densities in Fig. 2 we have chosen the value of activity Pe=8. It can be seen that the behaviour of particles under the presence of either a completely repulsive potential or a repulsive and attractive potential is considerably different. Common features in all three representations are a region where there are no particles due to the repulsiveness of the wall; a peak of the profile density that shows an accumulation of particles in that region of the space; a constant value of the profile density that corresponds to the volume's density, ρ_0.

If we compare Fig. 2 (a) and (b) we notice that the steeper the repulsive potential is, the more particles aggregate for a given value of activity. Conversely, at equilibrium particles do not aggregate. Thus, the probability density is constant in all the space except in the area where it decreases due to the repulsiveness of the wall.

Fig. 2 (c) shows that the probability density at a Pe=8 has negative values in a certain region of space. This is due to the fact that the second derivative of the potential is negative in a certain domain of positions because the potential has an attractive term. The attractive term also causes the friction coefficient Eq. (4) to be negative in certain region of space. There, the UCNA approximation we have used to derive the profile density is not valid because it requires the friction to be strictly positive. Apart from that, a negative friction lacks physical meaning. That is why the region where the profile is negative has no physical meaning and is a consequence of the type of potential which models the wall. We have studied the region of space where the friction coefficient is negative in order to clearly identify where UCNA is not valid and therefore to know the limitations of the model.

The peak in Fig. 2 (c) is narrower and higher than those in Fig. 2 (a) and (b). This is caused by the fact that aggregation in the case of the Lennard-Jones potential is not only due to activity but also has a contribution from the attractive part of the potential. Thus, particles will tend to accumulate themselves in the minimum of the well created by the attractive part of the potential. The peak showing the aggregation of particles will be narrower and higher than in the case of completely repulsive potentials. Between the density's peak and the density's negative region there is a domain where the profile's value is 0 and means that there are no particles. This is also caused by the attractive part of the Lennard-Jones potential which attracts particles to the minimum of the potential well leaving a space empty of particles. In this region the friction coefficient is positive, so the UCNA approximation is valid. Finally, when particles are subject to a Lennard-Jones potential they will tend to aggregate despite there is no activity, as a result of the attractive part of the potential. This is what shows the peak at the equilibrium profile density in Fig. 2 (c).

B. Adsorption

Adsorption is obtained by integrating over all the space the profile density of a system with a certain amount of activity minus the profile density of the same system at equilibrium, see Eq. (10). We have used Mathematica to numerically compute the integrals and to plot them as a function of activity. Hence, we have been able to study the dependence of adsorption on activity in a system subjected to a repulsive potential, Fig. 3 below.

In the case of the completely repulsive potentials, a certain amount of activity is needed to make particles aggregate, so there is no adsorption neither at equilibrium nor at small Péclet because repulsion due to the hard wall wins. The steeper the repulsive potential is the smaller the Péclet needs to be to produce adsorption. In other words, when the potential wall is steeper particles will find it easier to aggregate. This confirms what some authors refer to as the "attraction from repulsion".

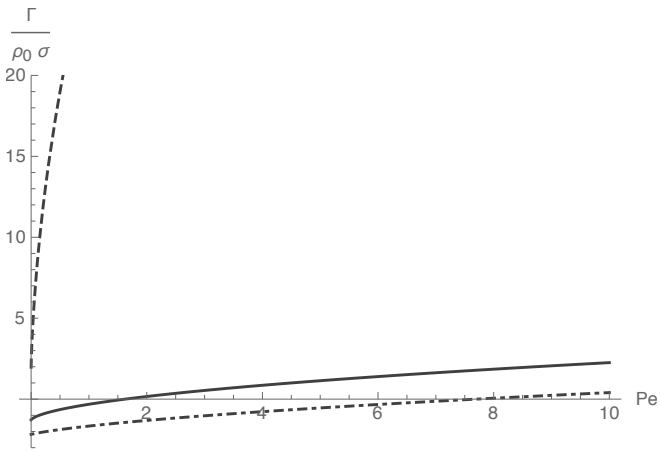

FIG. 3: Adsorption as a function of activity (Péclet). Full line: $u(x) = u_0\frac{1}{x^{12}}$; dashed-dotted line: $u(x) = u_0\frac{e^{-x}}{x}$; dashed line: $u(x) = u_0(\frac{1}{x^{12}} - \frac{1}{x^6})$.

In the case of the Lennard-Jones potential, adsorption grows much faster than in the other two cases as a function of the Péclet, Fig. 3 above. This is due to the contribution of the long-range attractive term that causes particles to aggregate despite there is no activity. This explains why at equilibrium particles will be able to aggregate and adsorption will be positive. This phenomena is in accordance with the peak of the profile density at equilibrium, Fig. 2 (c).

In Fig. 4 below we plot the logarithm of the adsorption caused by the three potentials as a function of the logarithm of activity and we compare it to the square root of the activity. We observe that the adsorption presents approximately the same dependence with the activity in the three cases. The $u(x) = u_0\frac{e^{-x}}{x}$ potential asymptotically grows with the $\sqrt{(Pe)}$. In the case of the other two

potentials, even though we cannot ensure that the adsorption grows exactly as the $\sqrt{(Pe)}$, it grows similarly to $\sqrt{(Pe)}$.

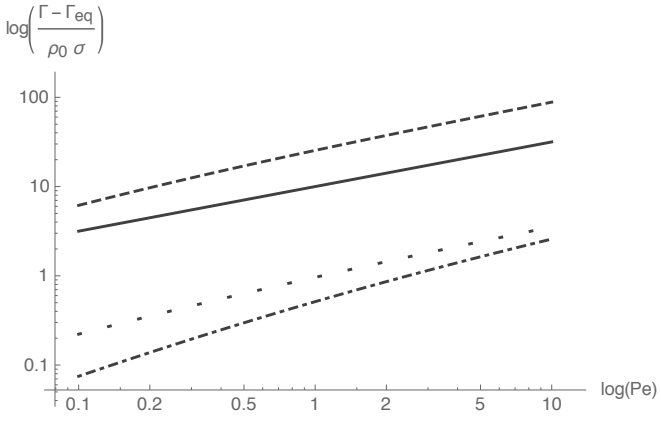

FIG. 4: Logarithm of the adsorption minus the adsorption in equilibrium as a function of the logarithm of activity (Péclet). Full line: $10\sqrt{Pe}$; dotted line: $u(x) = u_0\frac{1}{x^{12}}$; dashed-dotted line: $u(x) = u_0\frac{e^{-x}}{x}$; dashed line: $u(x) = u_0(\frac{1}{x^{12}} - \frac{1}{x^6})$.

IV. CONCLUSIONS

In this study we have analyzed the collective behaviour of a system of self-propelled particles subjected to a repulsive potential. In order to do so, we have worked with the Gaussian coloured-noise model to describe the active system. Applying the UCNA approximation we have obtained an analytic expression for the probability distribution function of the system under stationary conditions. With this, we have been able to use the single-particle distribution function to study the behaviour of active particles around a repulsive wall modelled by a repulsive potential.

We have seen that active particles tend to aggregate around repulsive objects although there are no attractive forces. We have modelled the repulsive objects using three different types of potential: two of them are strictly positive and the third one is a Lennard-Jones potential, which has a short-range repulsive term and a long-range attractive term. We can conclude that the more repulsive the potential is, the more particles tend to aggregate. In the case of the Lennard-Jones potential the attractive term of the potential favours the aggregation of particles near the repulsive wall.

The characteristic tendency of active systems to aggregate can be the cause of different physical phenomena. In this project, we have studied the adsorption as a function of activity. We can conclude that the more activity a system has the more adsorption there will be. It is important to mention that the type of potential applied influences the amount of activity needed to produce adsorption. For example, in the case of the Lennard-Jones potential, as the attractive term favours aggregation, less activity is needed to produce adsorption. Moreover, we have found that adsorption approximately grows as the square root of activity for the three potentials we have studied.

A further continuation to this work would be to add interactions between particles and study if under these conditions there is wetting. The study of the problem would be different in this case due to the fact that the particles would not stick to the wall homogeneously. Consequently, a different and more sophisticated treatment of the problem should be applied.

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