

Instituto Tecnológico y de Estudios Superiores de Monterrey

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## Induced Rotation of Ratchets in Passive Environments

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The committee members, hereby, certify that have read the thesis presented by **Yeray Cruz Ruiz** and that it is fully adequate in scope and quality as a partial requirement for the degree of Master in Nanotechnology.

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- Where I have consulted the published work of others, this is always clearly stated.
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---

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# **Dedication**

For those who come after.

# Acknowledgements

To my parents for their unwavering support, to my friends for making this journey easier, and especially to Dr. Antonio, who always believed in me and was an incredible mentor.

# **Induced Rotation of Ratchets in Passive Environments**

by

Yeray Cruz Ruiz

## **Abstract**

Swimming at the mesoscale has been a topic of interest for the past two decades because of the complexity of motion at a low Reynolds number, a regime where the viscous forces dominate over the inertial ones. The scallop theorem is a principle that follows these complex ideas and states that a scallop, which has only one degree of freedom, must be unable to have net displacement in this regime due to the lack of time-reversal symmetry of the Navier-Stokes equations. Indifferent to our mathematical understanding, nature was capable of creating biological beings that are able to displace under these circumstances by developing what we call nonreciprocal motion. The *Escherichia coli*, for example, has a flagellum that rotates in one direction, pushing the fluid backwards and therefore moving the bacteria forwards. Inspired by these ideas, researchers have taken interest in generating motion at those scales. One example are bacterial micromotors, where a dented ratchet is immersed into a bacterial bath where they convert energy from their surroundings into movement. This movement normally follows a ballistic trajectory and in time some of them, will collide into the ratchet transferring their kinetic energy, and therefore making the motor spin thanks to the geometry of the ratchet. Unfortunately, the nutrients they absorb will end and in time the system's medium will need to be replaced, stopping the whole process, therefore being an inefficient process. This is a type of active matter that gets energy from its medium. But, can we do the same with passive matter?

In this work, we analyze paramagnetic colloids, manipulated by an external precessing magnetic field. The system is confined between the  $z$  axis and presents periodic boundary conditions in  $x$ , and  $y$  axis. When multiple particles are present, dipole-dipole interactions arise, leading to either attraction or repulsion depending on their head-to-tail alignment. The particles' internal fields also rotate, dynamically altering their interactions over time. We observe that from 0Hz to 3Hz, the colloids form pairs and start rotating with a shared center of mass, whereas from 3.25 to 7Hz particles have a moment of repulsion, creating a neighbor exchange between different pairs, obtaining a ballistic trajectory. We observe that from 0Hz to 3Hz, the colloids form pairs and start rotating with a shared center of mass, whereas from 3.25 to 7Hz particles have a moment of repulsion, creating a neighbor exchange between different pairs, obtaining a ballistic trajectory. To investigate whether this motion can perform work, we place a ratchet-like object with different parameters amidst the particles.

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# **Part I**

## **Introduction**



# Chapter 1

## Introduction

The study of motion at the microscale sits between physics, chemistry, and biology, and has consequences both for basic science and for applications. At these scales, inertia can be ignored and viscous forces dominate. Random fluctuations from thermal noise also play an important role. How to control, rectify, and use this motion is one of the main questions in soft matter and statistical physics [1, 2]. Besides the theoretical interest, these ideas are useful for the design of microfluidic devices, targeted drug delivery, and even nanoscale engines.

Nature already provides many examples of how small systems can turn energy into motion. Inside cells, molecular motors like kinesin and dynein move cargo. Microorganisms such as *E. coli*, sperm cells, and algae have developed strategies to swim in viscous environments [3–5]. These observations gave rise to the field of *active matter*, which studies collections of self-driven units operating out of equilibrium [6–8]. The concept has expanded in recent years to cover emergent effects, such as topological flows in active materials [9].

One useful way to think about directed motion at this scale is through ratchets. These are asymmetric structures or potentials that turn random fluctuations into net motion, similar to Feynman’s ratchet thought experiment. Ratchets have been studied in both theory and experiments, leading to the broader field of Brownian motors [10, 11]. More recently, these ideas have been extended to active matter, where active Brownian particles can be rectified into directional transport [12–14].

Di Leonardo *et al.* (2010) harnessed the movement of living cells and showed that asymmetric microgears immersed in dense bacterial suspensions could rotate spontaneously, powered only by the activity of *E. coli* [15]. These bacterial ratchets combine nonequilibrium activity with geometric asymmetry to produce motion. Such systems point to possible uses in autonomous transport and mixing at the microscale. Also it has been studied how bacterium collisions with curved-geometry microstructures can exert net movement in these structures and how the curva-

ture of the surface can modify the speed of the structure [16].

Even with these advances, there are still open problems. Active matter is powerful but not always easy to control or keep stable, since living systems depend strongly on their environment [8]. Passive colloids are easier to handle in experiments but need external driving to move in a directed way. Magnetically driven colloids are promising in this respect because their interactions can be tuned, they are reversible, and they can be controlled externally. Experiments have shown magnetic colloidal carpets that propel and carry cargo [17], and other studies have revealed enhanced diffusion, synchronization, and bidirectional transport under confinement [18–20]. Still, the interplay between confinement, collective effects, and external driving is not fully understood.

This thesis looks at these questions by using numerical simulations of paramagnetic colloids under magnetic fields, with emphasis on confinement and ratchet effects. Simulations are useful because they allow us to test conditions that are hard to achieve in experiments and to separate the roles of noise, interactions, and driving. By studying transport properties, collective effects, and symmetry breaking, we aim to clarify how random microscopic motion can be rectified into useful work. The results connect to basic questions in nonequilibrium systems and may also guide the design of micro- and nanoscale devices, where controlled transport is essential.

The thesis is organized as follows. Part II reviews the theoretical background, including motion at low Reynolds number, Brownian noise, ratchet mechanisms, and the difference between active and passive matter. Part III describes the simulation methods, with focus on stochastic molecular dynamics. Part IV presents the main findings on confined colloidal dynamics and rectification. Finally, Part V summarizes the contributions and suggests future work.

# **Part II**

# **Background**



# Chapter 2

## Physics at the mesoscale

### 2.1 Low Reynolds number regime

At the mesoscale, where objects such as bacteria and colloidal particles operate, the physical world is governed by a regime in which viscous forces dominate over inertial ones. This regime is characterized by a small Reynolds number ( $Re$ ), a dimensionless quantity that compares inertial to viscous effects. Therefore, the force applied at that moment will describe the movement or displacement performed, not depending on any past force, this is a characteristic of an over-damped system. In his seminal lecture, Life at Low Reynolds Number, Purcell highlighted the surprising and often counterintuitive behaviors that emerge in such environments [1]. For instance, time-reversible motion — common at macroscopic scales — is ineffective for propulsion at low  $Re$ , necessitating non-reciprocal strategies like flagellar rotation or body undulation. This leads to the scallop theorem, that states that an animal with such degrees of freedom — in a viscous regime — will not have a net displacement.

This whole process can be described by the Navier-Stokes equation without the inertia terms, leaving us without any time depending terms as shown in Eq. (2.1).

$$-\nabla p + \eta \nabla^2 \vec{v} = 0 \quad (2.1)$$

This has been a topic of interest for researchers that are constantly looking for ways of transportation in those environments for specific tasks. Unfortunately this is not the only challenge we face when moving at the microscale.

## 2.2 Brownian Motion and Thermal Fluctuations

Even though this is a viscous regime, particles are not static. At small length scales, such as those of colloidal particles or bacteria, random thermal fluctuations become a dominant source of motion. This phenomenon, known as *Brownian motion*, was first explained quantitatively by Albert Einstein in 1905. He demonstrated that the irregular paths observed in microscopic particles suspended in fluid result from collisions with the molecules of the surrounding medium [2].

Einstein's work provided one of the first convincing arguments for the molecular nature of matter and led to a mathematical description of how these random movements accumulate over time. Specifically, he derived that the mean squared displacement (MSD) of a particle grows linearly with time:

$$\langle x^2(t) \rangle = 2Dt, \quad (2.2)$$

where  $D$  is the diffusion coefficient, a measure of how quickly particles spread out. Einstein further related this coefficient to measurable physical parameters through the expression:

$$D = \frac{k_B T}{6\pi\eta R}, \quad (2.3)$$

where  $k_B$  is Boltzmann's constant,  $T$  the absolute temperature,  $\eta$  the dynamic viscosity of the fluid, and  $R$  the radius of the spherical particle. This relation — often referred to as the *Einstein-Stokes equation* — is foundational in soft matter and colloidal physics.

In the systems considered in this thesis, Brownian motion plays a crucial role in the dynamics of passive colloids and must be accounted for even in the presence of external fields or active agents, such as bacteria.

While Einstein's formulation captures the long-term diffusive behavior of Brownian particles, it does not account for their instantaneous dynamics. To describe how particles move under both viscous damping and random thermal forces, we turn to a stochastic differential equation known as the *Langevin equation*.

### 2.2.1 Stochastic Representation

The Langevin equation [21] in one dimension, including inertial effects, damping, and thermal noise, can be written as:

$$m\ddot{x} = F - \lambda\dot{x} + \eta(t), \quad (2.4)$$

where  $m$  is the particle mass,  $\lambda$  is the damping coefficient, and  $\eta(t)$  is a stochastic force representing thermal noise. For simplicity, we write the velocity as  $v = \dot{x}$ , leading to:

$$m \frac{dv}{dt} = F - \lambda v + \eta(t). \quad (2.5)$$

Discretizing time with a small step  $dt$ , we apply the definition of a derivative:

$$m \frac{v(t+dt) - v(t)}{dt} = F - \lambda v(t) + \eta(t). \quad (2.6)$$

The thermal noise term  $\eta(t)$  is modeled as a Gaussian white noise process:

$$\eta(t) dt = g dW, \quad (2.7)$$

where  $dW$  is a Wiener process (increment of Brownian motion) such that:

$$\langle dW \rangle = 0, \quad \langle dW^2 \rangle = dt. \quad (2.8)$$

Solving for  $v(t+dt)$  gives:

$$v(t+dt) = v(t) + \frac{dt}{m}(F - \lambda v(t)) + g dW. \quad (2.9)$$

Now, assuming no deterministic force ( $F = 0$ ) — as is the case for free passive particles:

$$v(t+dt) = v(t) - \frac{\lambda dt}{m} v(t) + g dW. \quad (2.10)$$

Taking the expectation value (mean) of both sides:

$$\langle v(t+dt) \rangle = \langle v(t) \rangle - \frac{\lambda dt}{m} \langle v(t) \rangle + g \langle dW \rangle. \quad (2.11)$$

Since  $\langle dW \rangle = 0$ , the last term vanishes:

$$\langle v(t+dt) \rangle = \langle v(t) \rangle \left( 1 - \frac{\lambda dt}{m} \right). \quad (2.12)$$

In the limit of small  $dt$ , this leads to the differential equation:

$$\frac{d}{dt} \langle v(t) \rangle = -\frac{\lambda}{m} \langle v(t) \rangle, \quad (2.13)$$

whose solution is:

$$\langle v(t) \rangle = \langle v(0) \rangle e^{-\lambda t/m}. \quad (2.14)$$

This result shows that the average velocity of a particle in a viscous fluid decays exponentially due to damping. The characteristic timescale  $\tau = m/\lambda$  describes how quickly the particle forgets its initial velocity, after which the motion becomes diffusive.

### 2.2.2 Velocity Statistics and Energy Equipartition

To compute the variance of the velocity, we start again from the Langevin equation in discretized form, without external forces:

$$v(t + dt) = v(t) - \frac{\lambda}{m}v(t)dt + \frac{g}{m}dW. \quad (2.15)$$

Squaring both sides:

$$v(t + dt)^2 = \left[ v(t) - \frac{\lambda}{m}v(t)dt + \frac{g}{m}dW \right]^2, \quad (2.16)$$

$$\begin{aligned} &= v(t)^2 + \left( \frac{\lambda}{m} \right)^2 v(t)^2 dt^2 + \left( \frac{g}{m} \right)^2 dW^2 \\ &\quad - 2 \frac{\lambda}{m} v(t)^2 dt + 2 \frac{g}{m} v(t) dW - 2 \frac{\lambda g}{m^2} v(t) dW. \end{aligned} \quad (2.17)$$

Now we take the expectation value:

$$\begin{aligned} \langle v(t + dt)^2 \rangle &= \langle v(t)^2 \rangle + \left( \frac{\lambda}{m} \right)^2 \langle v(t)^2 \rangle dt^2 + \left( \frac{g}{m} \right)^2 \langle dW^2 \rangle \\ &\quad - 2 \frac{\lambda}{m} \langle v(t)^2 \rangle dt + 2 \frac{g}{m} \langle v(t) \rangle \langle dW \rangle - 2 \frac{\lambda g}{m^2} \langle v(t) \rangle \langle dW \rangle. \end{aligned} \quad (2.18)$$

Using the properties of the Wiener process:

$$\langle dW \rangle = 0, \quad \langle dW^2 \rangle = dt.$$

And neglecting second-order small terms ( $dt^2$ ), we obtain:

$$\langle v(t + dt)^2 \rangle = \langle v(t)^2 \rangle + \frac{g^2}{m^2} dt - 2 \frac{\lambda}{m} \langle v(t)^2 \rangle dt. \quad (2.19)$$

Taking the continuous limit:

$$\frac{d}{dt} \langle v(t)^2 \rangle = -2 \frac{\lambda}{m} \langle v(t)^2 \rangle + \frac{g^2}{m^2}. \quad (2.20)$$

This is a linear first-order ODE. Solving it with variation of constants yields:

$$\langle v(t)^2 \rangle = \frac{g^2}{2\lambda m} + D e^{-2\lambda t/m}. \quad (2.21)$$

As  $t \rightarrow \infty$ , the exponential term vanishes and we get the stationary value:

$$\langle v(\infty)^2 \rangle = \frac{g^2}{2\lambda m}. \quad (2.22)$$

From the equipartition theorem, we know that the average kinetic energy is:

$$\frac{1}{2}m\langle v^2 \rangle = \frac{1}{2}k_B T.$$

Therefore:

$$\langle v^2 \rangle = \frac{k_B T}{m}. \quad (2.23)$$

Matching this to our stochastic result:

$$\frac{k_B T}{m} = \frac{g^2}{2\lambda m} \Rightarrow g^2 = 2\lambda k_B T, \quad g = \sqrt{2\lambda k_B T}. \quad (2.24)$$

This defines the noise amplitude in terms of temperature, viscosity, and Boltzmann's constant.

### 2.2.3 Overdamped Dynamics and Diffusion

In the overdamped limit, inertia is negligible, so the Langevin equation becomes:

$$0 = F - \lambda \frac{dx}{dt} + \eta(t). \quad (2.25)$$

Solving for the velocity:

$$\frac{dx}{dt} = \frac{1}{\lambda}(F + \eta(t)). \quad (2.26)$$

For free diffusion ( $F = 0$ ):

$$\frac{dx}{dt} = \frac{1}{\lambda}\eta(t). \quad (2.27)$$

Using stochastic calculus with  $\eta(t)dt = gdW$ , we write:

$$x(t + dt) = x(t) + \frac{g}{\lambda}dW. \quad (2.28)$$

**Mean Position** Taking the expectation:

$$\langle x(t+dt) \rangle = \langle x(t) \rangle + \frac{g}{\lambda} \langle dW \rangle = \langle x(t) \rangle. \quad (2.29)$$

So the mean position remains constant in free diffusion.

**Mean Square Displacement (MSD)** Squaring the position update:

$$x(t+dt)^2 = x(t)^2 + 2\frac{g}{\lambda}x(t)dW + \left(\frac{g}{\lambda}\right)^2 dW^2. \quad (2.30)$$

Taking the expectation:

$$\langle x(t+dt)^2 \rangle = \langle x(t)^2 \rangle + 2\frac{g}{\lambda} \langle x(t) \rangle \langle dW \rangle + \frac{g^2}{\lambda^2} \langle dW^2 \rangle, \quad (2.31)$$

$$= \langle x(t)^2 \rangle + \frac{g^2}{\lambda^2} dt. \quad (2.32)$$

In differential form:

$$\frac{d}{dt} \langle x(t)^2 \rangle = \frac{g^2}{\lambda^2}. \quad (2.33)$$

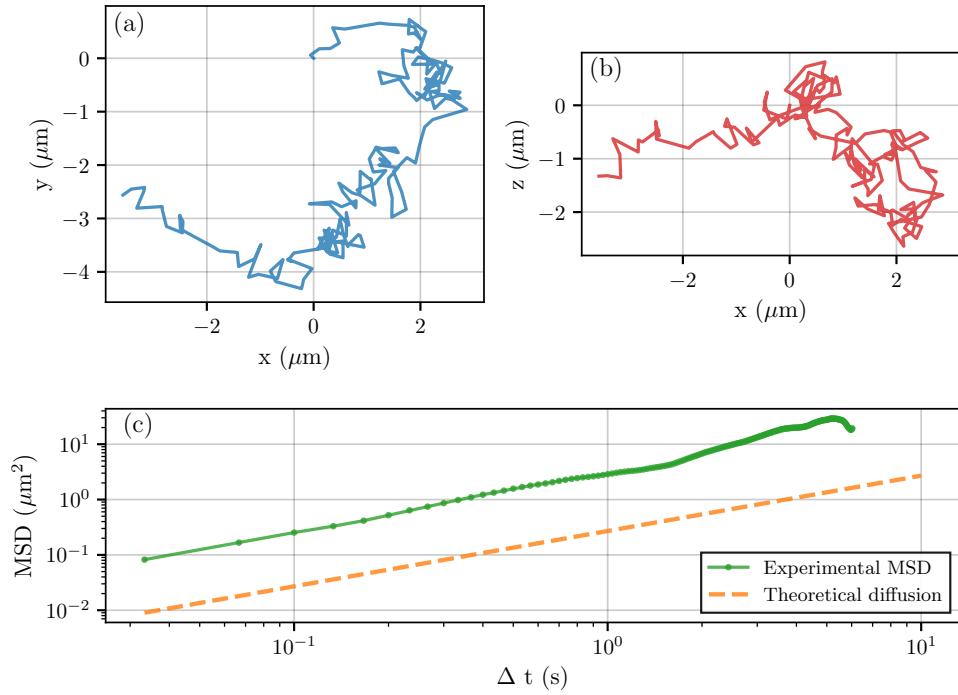
Using  $g^2 = 2\lambda k_B T$ , we substitute:

$$\frac{d}{dt} \langle x(t)^2 \rangle = \frac{2k_B T}{\lambda}. \quad (2.34)$$

Integrating gives the mean squared displacement (MSD):

$$\langle x(t)^2 \rangle = \frac{2k_B T}{\lambda} t. \quad (2.35)$$

This is the classical diffusion result, where the diffusion coefficient is  $D = \frac{k_B T}{\lambda}$ , consistent with Einstein's expression.



**Figure 2.1:** A colloidal particle undergoes random, thermally induced displacements in a fluid medium. **Panel a)** shows the trajectory of the particle. **Panel b)** shows the corresponding mean squared displacement (MSD) as a function of time, illustrating the linear relationship predicted by Einstein for diffusive behavior (orange) and the one obtained through a numerical simulation (blue).



# Chapter 3

## Ratchets and Rectification Mechanisms

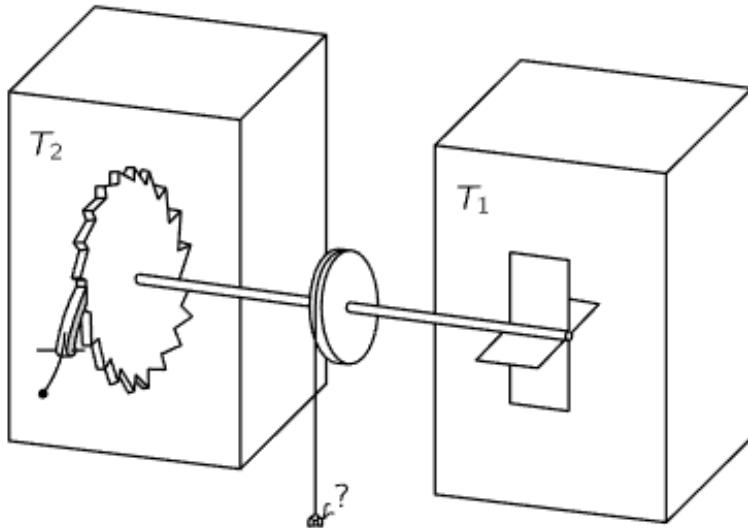
### 3.1 The Feynman-Smoluchowski ratchet

The inherent randomness of Brownian motion naturally leads to the question: can this disorder be transformed into order? In other words, can the random thermal motion of particles be used to produce directed movement or extract work? This question sits at the core of statistical mechanics and was famously explored by Richard Feynman in his lectures on physics, through a thought experiment known as the Feynman ratchet and pawl [22].

The Feynman ratchet consists of a set of vanes connected to a ratchet wheel, immersed in a fluid (Fig. 3.1). The idea is: random collisions from the surrounding molecules could push the vanes, but the pawl only allows rotation in one direction. At first glance, this asymmetric mechanism seems capable of converting random thermal motion into unidirectional rotation, apparently violating the second law of thermodynamics.

However, Feynman's analysis showed that when both the ratchet and the pawl are in thermal equilibrium with the same heat bath, the system cannot produce net work. The pawl itself undergoes thermal fluctuations and can occasionally lift off, allowing the ratchet to move backward. Over time, the forward and backward movements average out, and no net rotation occurs. This result reinforces the principle that thermal fluctuations alone cannot be rectified to perform work without a temperature gradient or an external energy input.

Despite this limitation, the Feynman ratchet introduced a powerful concept: asymmetry combined with non-equilibrium conditions can, in principle, produce directed motion. This idea is foundational in the study of Brownian motors, biomolecular machines, and active matter systems, including the systems explored in this thesis. In such systems, energy is continuously supplied, whether through bacterial metabolism or magnetic field modulation, creating the necessary non-equilibrium environment that allows motion rectification to occur.



**Figure 3.1:** Visual representation of the Feynman ratchet. Obtained from [22]

The failure of the Feynman ratchet in thermal equilibrium is intimately connected to another famous thought experiment: Maxwell’s demon. Both systems attempt to extract work from thermal fluctuations through selective processes—the ratchet through mechanical asymmetry, and the demon through information gathering.

Maxwell’s demon, proposed in 1867, imagines a microscopic being that can sort fast and slow molecules between two chambers, creating a temperature difference without apparent work. Similarly, the pawl in Feynman’s ratchet acts as a mechanical “demon,” attempting to select only forward fluctuations while blocking backward motion. However, both fail for the same fundamental reason: the cost of selection itself [23, 24].

Brillouin (1951) and later Landauer (1961) showed that Maxwell’s demon must expend energy to measure molecular velocities and erase information, with the minimum energy cost being  $kT \ln 2$  per bit erased. In the Feynman ratchet, the pawl must “decide” whether to allow motion, and this decision-making process—manifested as thermal fluctuations of the pawl itself—has an entropic cost that exactly cancels any work extracted [25, 26].

This connection reveals a deep principle: rectification requires either an information gradient (knowledge about the system) or an energy gradient (non-equilibrium conditions). As Parrondo and Español (1996) demonstrated, the Feynman ratchet can be viewed as an information engine where the pawl performs measurements on the ratchet’s position. When the pawl and ratchet are at the same temperature, the information gained equals the entropy produced, yielding no net work [27].

**Table 3.1:** Summary of operation of ratchet and pawl. Obtained from [22]

<b>Forward:</b>	Needs energy	$\epsilon + L\theta$ from vane. $\therefore$ Rate = $\frac{1}{\tau} e^{-(L\theta+\epsilon)/kT_1}$
	Takes from vane	$L\theta + \epsilon$
	Does work	$L\theta$
	Gives to ratchet	$\epsilon$
<b>Backward:</b>	Needs energy	$\epsilon$ for pawl. $\therefore$ Rate = $\frac{1}{\tau} e^{-\epsilon/kT_2}$
	Takes from ratchet	$\epsilon$
	Releases work	$L\theta$
	Gives to vane	$L\theta + \epsilon$

If system is reversible, rates are equal, hence

$$\frac{\epsilon + L\theta}{T_1} = \frac{\epsilon}{T_2}.$$

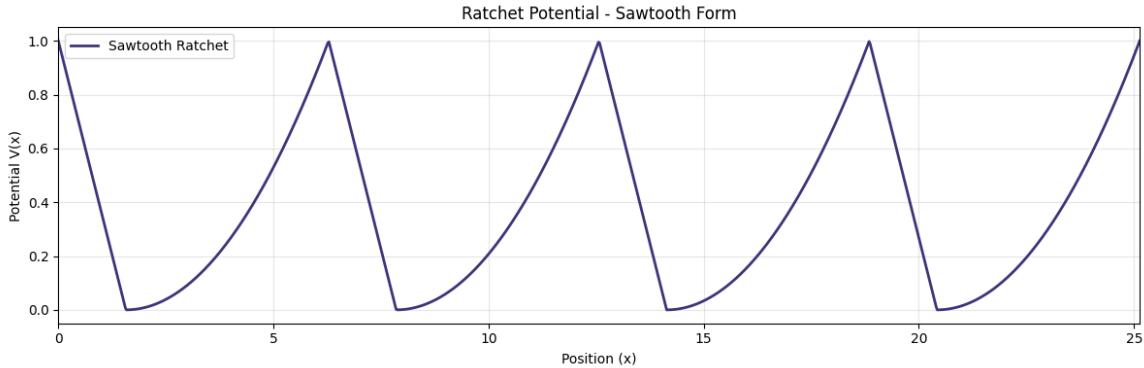
$$\frac{\text{Heat to ratchet}}{\text{Heat from vane}} = \frac{\epsilon}{L\theta + \epsilon}. \quad \text{Hence} \quad \frac{Q_2}{Q_1} = \frac{T_2}{T_1}.$$

## 3.2 Brownian ratchets

While Feynman's ratchet fails due to thermal equilibrium, rectified motion becomes possible when detailed balance is broken through external driving. Magnasco (1993) demonstrated this principle through the "rocking ratchet" mechanism [28]. In his model, a Brownian particle moves in an asymmetric periodic potential—essentially a sawtooth-shaped energy landscape with gentle slopes in one direction and steep walls in the other. The crucial innovation was applying an oscillating force  $F(t) = A \cos(\omega t)$  that rocks the potential back and forth. Although this force has zero time average—pushing equally left and right—the combination with the spatial asymmetry produces net directional motion. When the force tilts the potential forward, particles easily climb the gentle slopes and can overcome barriers. When tilted backward, particles encounter steep walls and remain trapped. This asymmetric response to symmetric driving breaks the forward-backward symmetry of thermal diffusion.

This mechanism differs fundamentally from Feynman's original ratchet: rather than attempting to rectify equilibrium fluctuations (which violates the second law), the rocking ratchet con-

tinuously injects energy through the oscillating force. The time-dependent driving maintains the system far from equilibrium, enabling the spatial asymmetry to generate directed transport. This principle—that asymmetry plus non-equilibrium driving yields rectification—underlies numerous biological processes and provides the theoretical foundation for the magnetically-driven ratchets explored in this thesis.



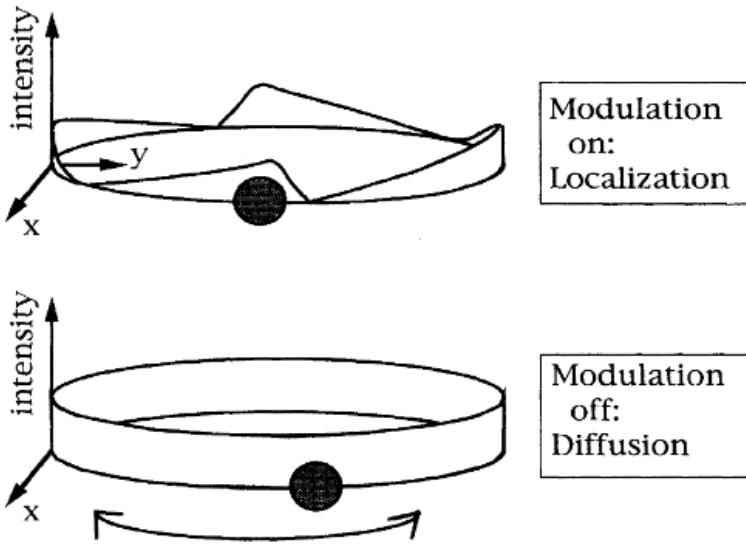
**Figure 3.2:** Example of a commonly used ratchet potential.

Following Magnasco’s rocking ratchet where an oscillating force drives particles in a static potential, Ajdari et al. (1994) analyzed rectification in periodic structures with either spatial or temporal asymmetry [29]. Using a sawtooth potential with asymmetric slopes (steep of height  $\epsilon/a$  and gentle of  $\epsilon/b$ ), they identified distinct transport regimes as a function of the AC force amplitude  $\gamma$ .

For small forces  $\gamma < \epsilon/a$ , particles remain trapped. In the intermediate regime  $\epsilon/a < \gamma < \epsilon/b$ , rectification occurs as particles can climb the gentle slope but not the steep one, yielding either integer velocities  $V = n$  when particles fully relax between cycles, or rational velocities  $V = n - 1/(m + 1)$  when incomplete relaxation creates a periodic pattern over multiple cycles.

This concept was later demonstrated experimentally by Faucheux et al. (1995), who created an “optical thermal ratchet” using focused laser beams [30]. To generate a circular trap without introducing external forces, they passed the laser through a plate to create circular polarization, maintaining constant laser intensity along the circular path. By rotating the laser frequency fast enough, particles could not experience any directed force from the beam itself, allowing them to move freely, then modulated the beam intensity to create an asymmetric potential mimicking a ratchet shape, as shown in Figure 3.3. They observed that particles localized in potential minima when the modulation was turned on, while for sufficiently long periods, particles moved either backward or forward with equal probability.

A different approach was developed by Lee et al. (2004), who employed holographic optical

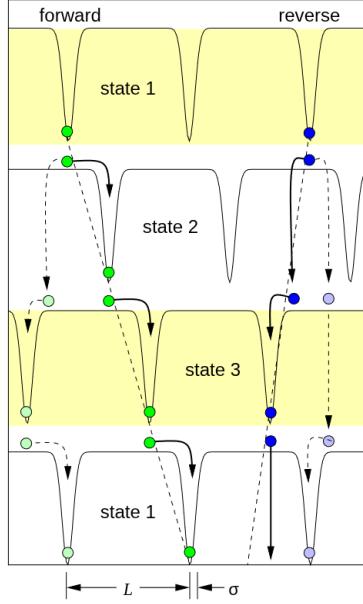


**Figure 3.3:** When the modulation is on, the beam intensity follows the shape of a ratchet potential with 4 periods per cycle. When the modulation is off, the intensity remains constant, allowing particles to diffuse freely. Obtained from [30].

trapping with a symmetric potential [31]. Their system consisted of discrete optical tweezers functioning as potential wells. Between each state, particles are released and free to diffuse, nevertheless they can rapidly jump between adjacent traps. Using this methodology, they achieved net particle displacement in one direction, as illustrated in Figure 3.4. Remarkably, when they reversed the direction of well displacement, particles followed the trap movement in the opposite direction. Due to this predictable response to trap motion, they named this system a "deterministic thermal ratchet."

Lebedev et al. (2009) modified this approach by using three linearly polarized beams acting only in the  $xy$ -plane, as shown in Figure 3.5 [32]. They applied forces to particles by phase-modulating two of the three lasers, which shifts the entire optical lattice. The modulation was generated using RF generators to produce potentials  $V_x$  and  $V_y$ . The sum  $V_x + V_y$  served as the input signal for beam 2, while the difference  $V_x - V_y$  was used for beam 3, creating the rocking forces. They studied this system using ultracold rubidium atoms as test particles. To track the atomic positions, they employed a CCD camera to determine the center of mass of the atomic cloud.

In their first experiment, they applied a biharmonic drive along only one axis. As expected, the system reduced to a one-dimensional harmonic ratchet, and they observed directed particle motion along the axis of the applied biharmonic force. In subsequent experiments, they applied

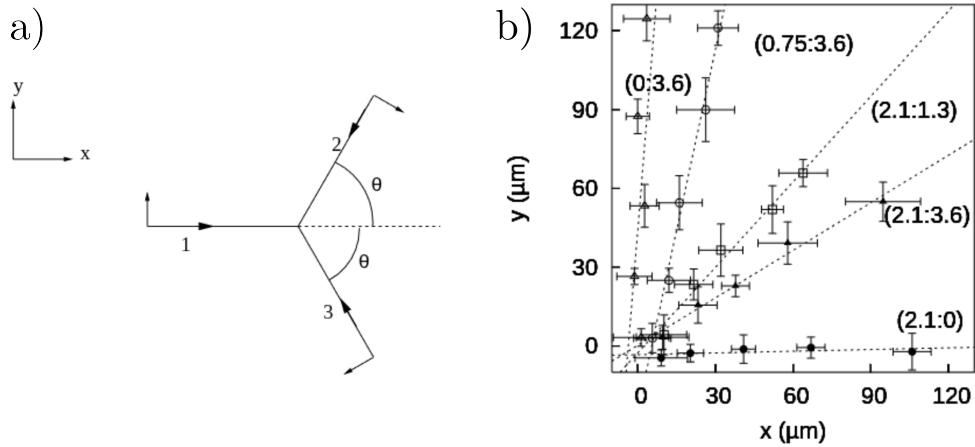


**Figure 3.4:** Discrete pattern of optical traps with displacement in one direction, minimum width of  $\sigma$  and a maximum width of  $L$ . Obtained from [31]

harmonic drives along both axes, with one frequency being twice the other. Their results showed that particles experienced directed motion along the axis with the faster harmonic, while motion along the other axis remained diffusive. In their final experiment, they applied biharmonic drives simultaneously along both axes to investigate whether directed transport could be achieved in two dimensions. By varying the relative weights of the forces along each axis, they demonstrated that it was possible to control the atomic displacement and direct atoms to specific target positions as shown in Figure 3.5 a).

Following the same lattice-based approach, Arzola et al. (2017) successfully recreated all five two-dimensional Bravais lattices using computer-generated holographic optical micromanipulation [33]. Their potential consisted of Gaussian wells distributed along a primary lattice, combined with a shifted replica of the same lattice with a reduced depth factor,  $Q$ , compared to the original. The asymmetry of the resulting potential depended directly on both the depth factor  $Q$  and the displacement between the original and replica lattices. They implemented the rocking mechanism by moving the particle cell along one axis.

The researchers performed three main experiments to validate their results, each with three different diffusion parameters (including no diffusion as one condition), calculating the current in the x and y axes with respect to the amplitude of movement. In the first experiment, they set the asymmetry parallel to the rocking force. They observed that since the wells were aligned with



**Figure 3.5:** **Panel a)** Lattice beam configuration in the xy plane.  $\theta = 60^\circ$ . **Panel b)** Position of the atomic cloud center of mass at different instants and forces when applying biharmonic at the same time in xy-plane. Obtained from [32].

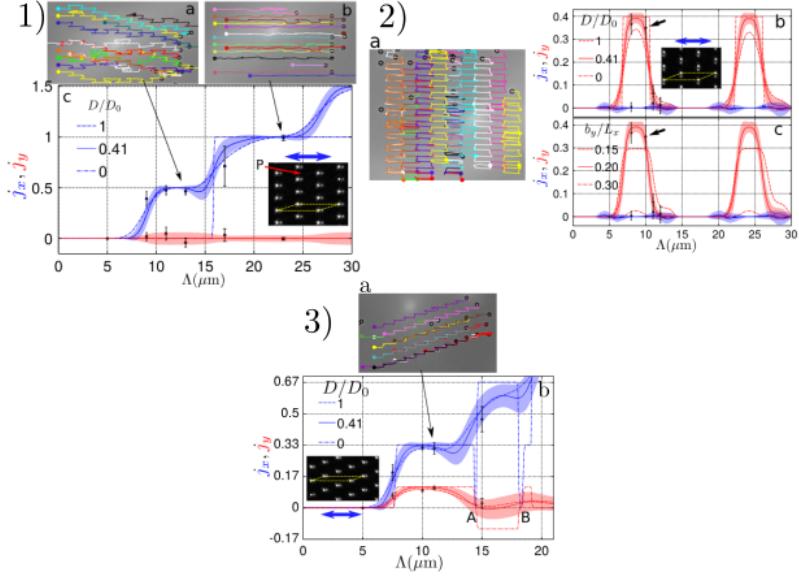
the particle movement, particles tended to move in the direction of the force, traveling from well to well, while experiencing no movement in the perpendicular direction. Current was present along the entire amplitude range.

The second experiment positioned the asymmetry perpendicular to the rocking force direction, yielding interesting results. Similar to the first experiment, current appeared along only one axis (the asymmetry axis), but the current behaved like a Gaussian bell curve. When the rocking movement amplitude approached the asymmetry lattice spacing, particles only moved back and forth between two wells in the x direction, experiencing no current in the y axis.

For the final experiment, they examined how the system behaved under a combination of both previous configurations. They created an oblique lattice with the asymmetry aligned with the rocking force direction, producing an oblique particle current. The results were essentially a combination of the two previous experiments: at certain amplitudes, current appeared in both axes, but as amplitude increased, the y-axis current decreased while the x-axis current increased. The results for each experiment can be seen in Figure 3.6.

Feynman demonstrated that a purely thermal Brownian ratchet cannot generate directed motion due to the second law of thermodynamics. However, introducing specific conditions to break symmetry has proven ideal for bypassing these limitations.

One successful approach to achieving this symmetry breaking involves rocking ratchets, where an external periodic drive is applied to an asymmetric potential. Previous experiments have demonstrated the potential of optics to create such asymmetries with high precision and



**Figure 3.6:** **Panel 1)** Experimental trajectories for assymetry parallel to rocking movement with a) rocking amplitud of  $13 \mu\text{m}$  and b)  $23 \mu\text{m}$ .c) Graphs of simulations showing the current for each axis. **Panel 2)** Experimental trajectories for assymetry perpendicular to rocking movement with a) rocking amplitud of  $10 \mu\text{m}$ . b) and c) Shows the current for each axis with different lattice parameters. **Panel 3)** Experimental trajectories for oblique lattice with assymetry perpendicular to the rocking movement with a) rocking amplitud of  $11 \mu\text{m}$ . b) Current for each axis. Obtained from [33].

control. While obtaining directed motion at the microscale remains challenging, by applying these symmetry-breaking parameters it becomes possible not only to overcome thermal noise but to harness it for directional transport. Unfortunately, as shown in previous works, implementing these systems often requires specific and sophisticated experimental setups. Interestingly, nature has already developed an alternative solution by creating matter capable of self-propulsion, known as active matter, which achieves directed motion through entirely different mechanisms.

# Chapter 4

## Active Matter Systems

### 4.1 Fundamentals of Active Matter

The definition of active matter is not always the same across the literature. Some authors describe it in a broad way, emphasizing that the key element is the continuous intake and dissipation of energy by each unit, which allows them to remain out of equilibrium and sustain motion or internal stresses. Reviews often highlight internally driven systems—such as cytoskeletal extracts, swimming microorganisms, or synthetic colloids—as the most representative examples of active matter [5, 6, 8].

Other authors focus more specifically on self-propulsion at the particle level as the defining feature. This perspective is useful for distinguishing active systems from those whose dynamics are mainly caused by externally imposed forces. For example, in vibrated granular monolayers, asymmetric grains can display self-propelled trajectories and flock-like patterns and are sometimes described as active. In contrast, symmetric grains that only move in a directed way because of an asymmetric boundary, such as a sawtooth channel, are better classified as externally driven rather than active [34–36].

There is also a difference when considering individual vs. collective behavior. Some colloids appear passive when studied alone, but when interactions are taken into account, they can exhibit genuinely non-equilibrium collective phenomena. Examples include motility-induced phase separation (MIPS), defect-mediated flows in active nematics, and other emergent patterns normally linked with active matter. For this reason, several reviews describe active matter not only in terms of single-particle propulsion but also in terms of its collective stresses and patterns [37, 38].

Simple theoretical models have played a crucial role in understanding active matter. One of the best-known examples is the Vicsek model, which shows how local alignment rules together with noise can lead to large-scale collective motion from basic self-driven units [39, 40]. At the

level of single particles, the Active Brownian Particle model is a common way to study colloidal swimmers. In this model, motion is explained by a constant propulsion force, combined with random changes in orientation resulting from rotational diffusion [41, 42].

More recent works point out that definitions have evolved over time and suggest clarifying criteria such as whether the drive is internal or external, whether the system is dry or wet (momentum non-conserving or conserving), and whether the energy input acts at the particle level. Some surveys even propose that researchers explicitly state their working definition depending on the context of their problem [43, 44].

**Working definition.** In this thesis, we define active matter as:

systems composed of units that continuously draw energy at the particle scale and convert it into mechanical work, generating persistent stresses or self-propulsion, and sustaining non-equilibrium collective dynamics.

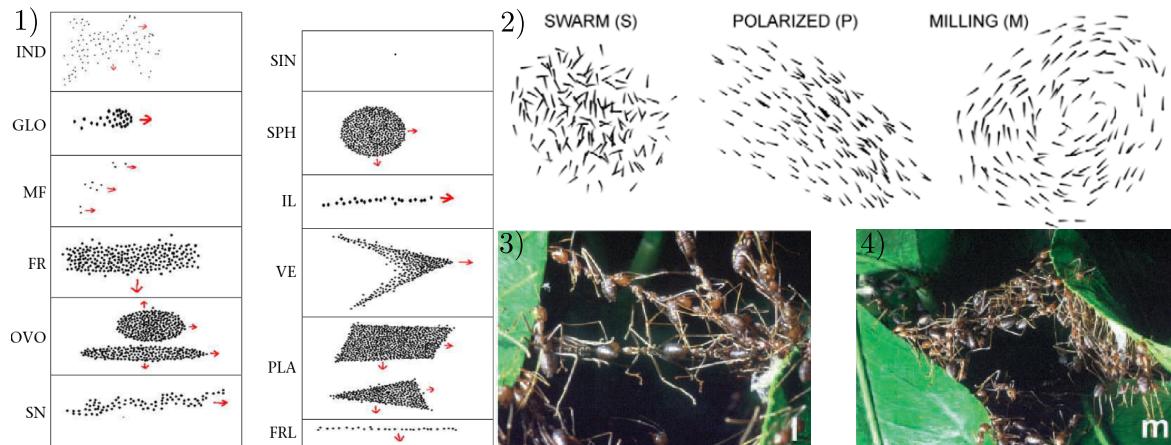
This definition includes both biological and synthetic systems (such as bacteria, cytoskeletal extracts, and Janus colloids) but excludes setups where directed motion arises only from externally imposed vibrations or asymmetric boundaries without particle-level energy input—for example, symmetric grains transported by a sawtooth channel [11, 45].

We will first present some macroscopic examples that show universal principles of self-organization, and then move to the microscopic cases most relevant to this work—active colloids, run-and-tumble swimmers, and active nematics—where thermal noise and low-Reynolds-number hydrodynamics play a dominant role.

## 4.2 Macroscopic Agents

Examples of active matter can be observed at plain sight in the macroscopic world. A flock of birds, for instance, is considered active matter because each bird is capable of self-propulsion. Unlike microscopic systems, they are not significantly affected by the thermal noise of their medium—in this case, air. A computational study by Reynolds (1987) modeled flocking behavior in birds by treating each individual as an autonomous agent whose trajectory was influenced by its local environment and neighboring individuals [46].

Reynolds introduced three fundamental rules governing flocking behavior: separation (collision avoidance), alignment (velocity matching with neighbors), and cohesion (attraction toward the average position of neighbors). This work laid the foundation for understanding how simple local interactions can give rise to complex patterns of collective motion.



**Figure 4.1:** **Panel 1)** Example of different formation of birds deppending predation risk, obtained from [49]. **Panel 2)** Different formation of schooling fish, obtained from [54]. **Panel 3) - 4)** Aggregation of ants forming a bridge, obtained from [55].

Over time, further developments in the study of group dynamics have incorporated methods such as dynamical maximum entropy to predict the alignment of ordered groups [47]. Following a maximum entropy approach, network reshuffling was later studied [48]. These behaviors, however, can change due to external factors, such as predation risk, which influences the formation and density of flocks [49]. In addition, individual characteristics can also affect collective behavior [50].

There are also self-organized groups of smaller flying animals whose collective behavior is even more complex than that of larger species. For example, bees are capable of dividing labor as a result of social interactions among individuals [51]. Remaining within the field of insects but shifting to a solid medium, ants exhibit similar patterns of labor division. Their organization can transition between ordered and disordered states depending on colony size. The disordered state typically occurs when the number of foraging ants is small, due to the infrequent discovery of food [52]. However, even when the colony is large enough to sustain a greater number of foragers, problems can still arise. In particular, some ants may remain stationary, occupying tunnels and thereby reducing the overall flow rate [53].

Another characteristic that arises from self-organization in ants—one not possessed by all animals—is their ability to self-assemble to perform specific tasks. Examples include the formation of rafts, bridges, or columns, where each individual uses its legs or jaws to grasp another and remains in place until the collective goal is achieved. Naturally, certain factors influence these self-assemblages, one of the most significant being colony size [55]. Interestingly, these structures posses some viscoelastic properties, when applied a certain stress, they tend to return

to their original place, resulting in an elastic behavior, at the same time they adapt a viscous behavior due to objects being able to sink in the aggregation, the same way they would do in a viscous fluid [56]. This opens the possibility for ants to be used as smart materials.

There are also animals that form groups while inhabiting more complex environments, such as water. Regardless of the medium, different species often display similar behaviors and dependencies. For example, the dynamics of schooling fish can be predicted, typically resulting in three main configurations, with variations depending on group size [54, 57, 58].

These are just few examples of large animal groups that, interestingly, share common characteristics of self-organization. This process begins at the level of the individual but emerges as a collective, temporary order through direct or indirect interactions among organisms, ultimately allowing them to achieve a common goal [59].

The study of macroscopic agents reveals that self-organization is not limited to large animal groups. At smaller scales, microscopic agents such as bacteria, colloidal particles, and artificial swimmers also exhibit analogous self-organized behaviors, although these are driven by different physical principles, including thermal noise and low-Reynolds-number hydrodynamics.

### 4.3 Microscopic agents

As discussed in the previous section, the term active matter is not limited to microscopic systems but also applies to animal groups. However, the focus of this thesis will be on the former.

We have already defined how a passive brownian particle acts, therefore let us review the key difference of active and passive ones. Passive particles undergo mere diffusion motion, whereas active follows stochastic differential equations according to [60]:

$$\frac{d}{dt}x(t) = v \cos \varphi(t) + \sqrt{2D_T}W_x, \quad (4.1)$$

$$\frac{d}{dt}y(t) = v \sin \varphi(t) + \sqrt{2D_T}W_y, \quad (4.2)$$

where  $W_x$ , and  $W_y$  represent their corresponding Wiener process, and  $v$  is the mean velocity. As stated before, if

$$\lim_{v \rightarrow 0} v \cos \varphi(t) + \sqrt{2D_T}W_x, \quad (4.3)$$

then the motion is merely diffusive and the particle is characterized as passive brownian particle.

However, they also exhibit some randomness; it is rare for them to move exactly in a straight line, and this is where chirality comes into play. There are three different forms of asymmetry:

rotational, reflexional, and a combination of the two. If a particle does not meet any of the three criteria, then the particle is not symmetric in any aspect. Chirality is actually the name for a non-reflexive-symmetric particle, as exemplified by our hands, from which the actual word originates [61].

Therefore adding an important third term for the rotational diffusion given by:

$$\frac{d}{dt}\varphi = \sqrt{2D_R}W_\varphi. \quad (4.4)$$

Despite this limitations, researchers have been developing new methods to achieve self-propulsion that mimic natural processes. In the following subsections, we will introduce a few examples of different systems that have been created, as well as organic ones.

### 4.3.1 Artificial Systems

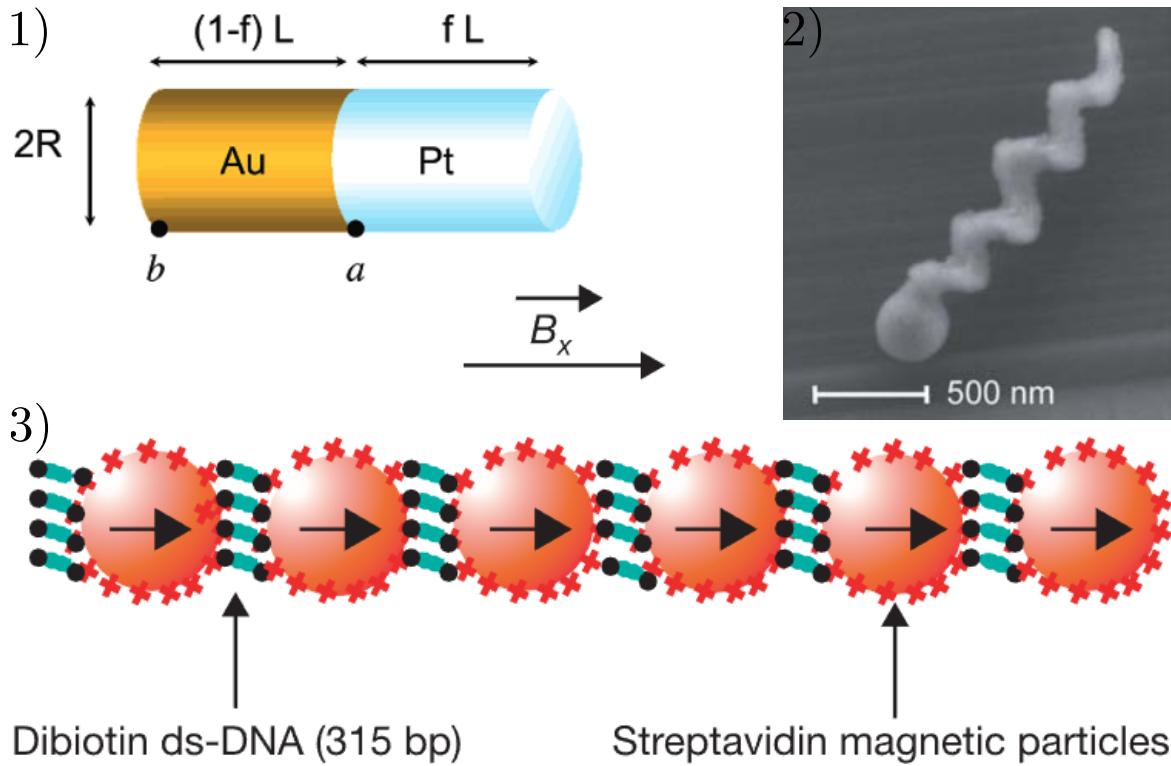
As discussed in Section 4.1, the definition encompasses various mechanisms of self-propulsion, and the list and discoveries are extensive.

Take, for example, *PDMS platelets coated with Pt* by Ismagilov et al. (2002), it appears to be the first realization of this method. The motion itself is not performed by the particle, but by the layer of platinum (catalyst). This is a chemical reaction where the components move by the releasing of bubbles produced when a liquid (hydrogen peroxide) breaks down with the help of a catalyst [62]. If we examine the definition of a catalyst, this one does not seem to be affected by the reaction; therefore, the movement would occur indefinitely. In fact, under the experiment's conditions, they achieved an uninterrupted motion of approximately 2 hours.

In the movement of the particles, they saw that they do not move in a straight line but rather in a circular manner, which is due to the chirality. They observed this behavior in all the particles; however, it was not completely identical.

This experiment opened up the possibility of different setups; the previous one, where plain plates were used, raises a question: Does this behavior depend on the shape of the particle? Paxton et al. (2004) did a similar experiment with a slightly different setup, utilizing rods with a diameter of 370 nm, with 2 stripes of platinum and gold, each one of 1 μm long in the direction of the long axis. Recalling the previous experiment, platinum is a catalyst for hydrogen peroxide; however, the twist here is that gold is not [63]. Although the setup was similar, using the same chemicals, the results differed. They observed that the rods had a tendency to move along their elongated section, particularly where the platinum was located, yielding a different result from the previous experiment, where the particle moved in the opposite direction to the platinum.

Not so much time later, Dreyfus et al. (2005) claimed that at that point, there was no artificial swimmer that had a *controlled swimming motion* [64]. They combined organic and artificial ele-



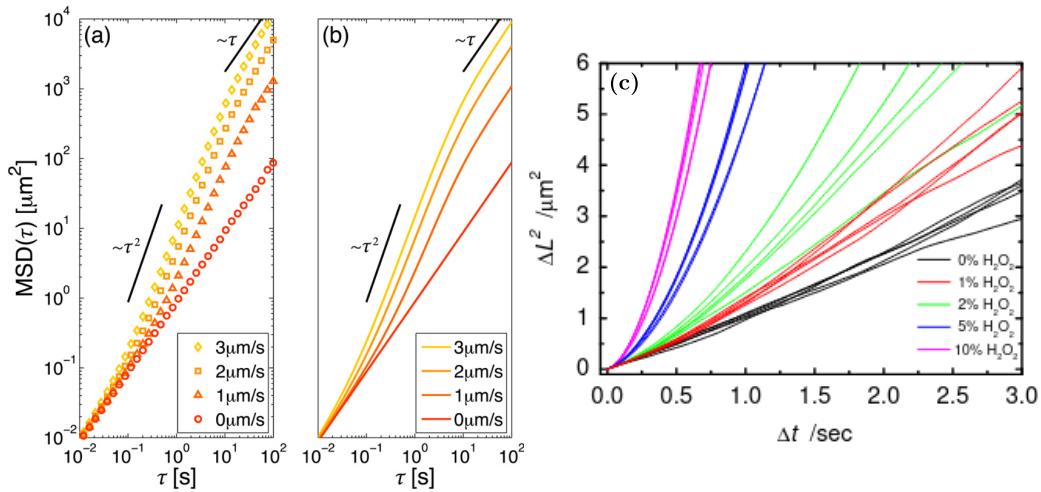
**Figure 4.2:** **Panel 1)** shows the configuration of nanorods of Gold (Au) and Platinum (Pt), obtained from [63]. **Panel 2)** Shows a Silicon Dioxide nan rod, obtained from [65].**Panel 3)** shows a chain of red blood cells linked with superparamagnetic filaments, obtained from [64].

ments; they used superparamagnetic filaments that respond to a magnetic field. These filaments are attached to a red blood cell, joining multiple to obtain a chain. To control the behavior of the filaments, they used two magnetic fields: a constant field parallel to the filament and a sinusoidal field perpendicular to the filament. With this approach, they were not only able to control the direction but also the speed by adjusting the frequency of the sinusoidal field, and the direction towards the parallel field.

However Howse et al. (2007) established the experimental basis for active Brownian particle dynamics by studying self-motile colloidal particles that use chemical reactions catalyzed on their surface to achieve autonomous propulsion. They demonstrated that at short times, these particles exhibit substantial directed motion with velocity dependent on fuel concentration, while at longer times, the motion transitions to a random walk with enhanced diffusion coefficients. This work provided a comprehensive experimental validation of the theoretical active Brownian particle model and established the standard mathematical framework for describing such systems through stochastic differential equations [66, 67]. These were done by coating polystyrene sh-

peres with a layer of platinum, the same process as the plates and the nanorods, which will be the responsible of the propulsion method, nontheless, this is not inherently of the particle's shape, there have been assymetric artificial particles with an *L* shape that undergoes the same behavior [68].

Figure 4.3 helps visualize how the motion varies according to their velocity. When the average velocity is zero, the linear behavior of the MSD represents a diffusive behavior, whereas when it is different it is considered to be ballistic.



**Figure 4.3:** MSD for brownian particles with different velocites. **Panel a)** shows the result from simulations. **Panel b)** shows the theoretical calculation, obtained from [60]. **Panel c)** MSD for different velocities of polystyren spheres for different concentrations of Hydrogen Peroxide, obtained from [66].

Tierno et al. (2008) proposed a new mechanism where two linked paramagnetic colloidal particles of different sizes, need no deformation for propulsion [69]. Their setup consists of colloids dispersed in water above a flat glass plate in the presence of a precessing magnetic field parallel to the plate. Here, the plate plays an important role for the rotating colloids, due to the dynamics it has when particles are near a boundary. When the smaller one is near the glass, the viscosity increases, resulting in lateral translation of the small colloid.

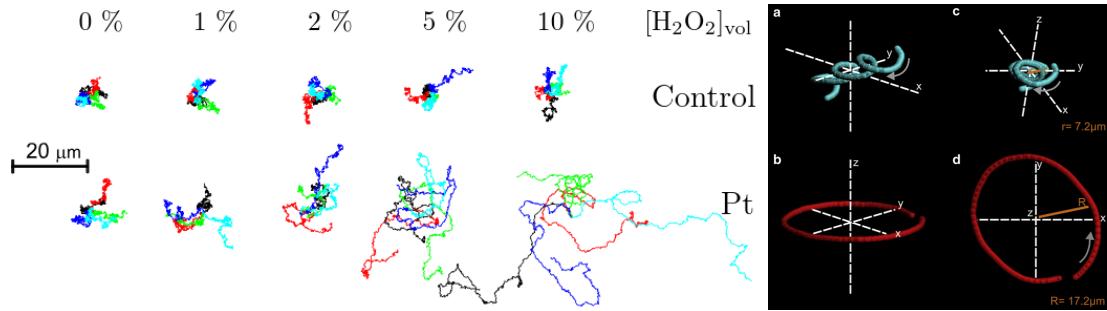
Based on the premise of biomedical purposes, Ghosh et al. (2009) proposed a system where helical screw nano propellers' control is so precise that it can be manipulated with a tolerance of microns [65]. Their size is approximately 200-300 nm, making them ideal for navigating confined spaces inside and not being intrusive. They are driven by a magnetic field. Half of the helices are covered with cobalt, which has ferromagnetic properties, and then placed between two electromagnetic poles with a homogeneous precessing magnetic field, making the magnetic

moment align with their long axis. Since the ferromagnetic part has a natural magnetic moment, it aligns with the external field, causing it to rotate along the helix. For each rotation, the particle moves either forward or backward, depending on certain values of the helix's geometry.

### 4.3.2 Natural Systems

We note how researchers have developed numerous strategies to achieve what was already accomplished by nature over a long period. In this section, we will present some examples of biological agents that inspired this thesis.

In a research by Corkidi et al. (2008) spermatozoa behavior was studied in a 3-dimensions space mimicking their real environment in search for eggs, what they found was a helical trajectory, shown in Figure 4.4, being a pretty similar response, and obtaining a non-space dependant behavior [70].



**Figure 4.4:** Trajectories of polystyrene platinum layered sphere particles for different peroxide concentrations, obtained from [66]. Trajectory of the spermatozoa for **a,c** free space, and **b,d** confined 2-dimension space. Obtained from [70].

It seems we cannot avoid randomness even for active particles, in a regime where viscous forces are predominant, a little symmetry breaking noise that perturbs the direction of the particle can make the origin of a random walk, but nature, as always, has evolved elegant solutions to this challenge through various biological mechanisms. A prime example is *E. coli*, which employs helical flagella that can rotate both clockwise and counterclockwise, generating two distinct types of motion that researchers have termed "run"—swimming in a straight line—and "tumble"—rotation in a random direction. This behavior also depends on the medium's viscosity and random fluctuations [71]. The way *E. coli* achieves a "run" state is due to their flagella which has two different motions for its power and recovery strokes, simulating those of a human breast strokes, although a tumble state is unavoidable, it is a great opportunity to harness the directed motion of the particle and see if it is possible to obtain work of it.

Marine bacteria are another example of an organic microswimmer; this can obtain individual speeds ten times faster than that of E. Coli ( $40 \mu\text{ms}^{-1}$ ) [72, 73]. Marine bacteria have a similar mechanism as E. Coli, responding to amino acids utilising a run and reverse motion, different from the run and tumble, allowing them to stop and reverse their direction, making it more efficient reaction [74]. However, since this bacterium is often found in the ocean, where its nutrients are constantly in motion, a study by Barbara et al. (2002) aimed to investigate how it would react to obtain its nutrients [75]. Interestingly, thanks to the motion system, marine bacteria were able to turn multiple times in the direction of the nutrients, thereby tracking them unequivocally.

Another remarkable example of biologically active matter is the green alga *Chlamydomonas reinhardtii*. This unicellular microorganism swims using two anterior flagella that beat in a breaststroke-like motion, propelling the cell forward through the water. Unlike bacteria, which rotate their helical flagella, *Chlamydomonas* relies on the coordinated motion of paired flagella, leading to straight swimming when both are synchronized and to turning when the coordination is lost [76]. Because of this, *Chlamydomonas* is often used as a model organism to understand how eukaryotic cells achieve motility at low Reynolds number.

Another type of biological microswimmer is found in protozoa such as *Paramecium*. These ciliates are covered with thousands of cilia that beat in a coordinated manner, producing smooth gliding motion through viscous fluids [77]. Cilia not only enable propulsion but also allow *Paramecium* to sense and respond to chemical gradients in their environment, demonstrating an early form of mechanosensory feedback in microswimmers.

At a different scale, immune system cells, such as neutrophils, also display active motility, although they crawl rather than swim. Neutrophils move by extending actin-rich protrusions (lamellipodia) and contracting their cell body, enabling them to pursue pathogens in tissues [78]. While their propulsion mechanism differs from that of flagellated or ciliated organisms, neutrophils still exemplify how living systems consume energy internally to generate directed motion.

These diverse biological strategies demonstrate how nature has evolved multiple solutions to achieve motion in environments dominated by viscous forces. Each of these mechanisms—flagellar beating in algae, ciliary coordination in protozoa, or actin-driven crawling in immune cells—highlights the central role of active matter principles in biology. But, is their locomotion enough to produce work?

## 4.4 Obtaining Work from Active Matter

A fundamental question in active matter research is whether the continuous energy consumption and motion of biological microswimmers can be harnessed to perform useful work. In nature, molecular motors such as kinesin, dynein, and myosin already accomplish this inside cells, driving processes like vesicle transport, muscle contraction, and chromosome segregation. Inspired by these nanoscale examples, researchers have investigated whether intact organisms at the microscale can be used as biological engines outside their natural environments [79].

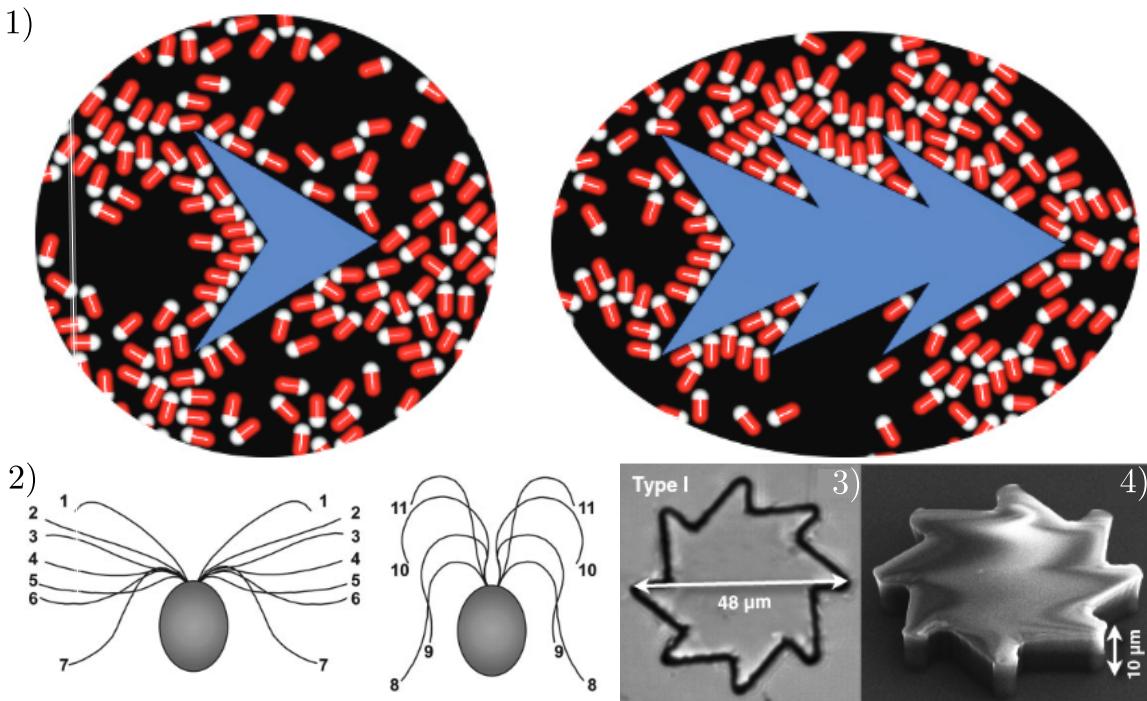
One particularly illustrative example comes from the work of Weibel et al. (2005), who introduced the concept of “*microoxen*” — motile cells of the green alga *Chlamydomonas reinhardtii* [80]. In their study, the authors exploited the flagellar beating of *Chlamydomonas* to transport microscale loads such as polystyrene beads. By chemically attaching the beads to the cell wall, these algae were able to carry particles 1–6  $\mu\text{m}$  in diameter without significantly reducing their swimming velocity (100–200  $\mu\text{m/s}$ , similar to unmodified cells).

An important feature of this work was the ability to control and manipulate the cells. Because *Chlamydomonas* exhibits positive and negative phototaxis [81], its direction of motion could be guided in microfluidic channels by alternating visible light sources. This allowed them to steer cargo-carrying cells back and forth repeatedly over distances of up to 20 cm. Moreover, by including a *photocleavable chemical linker* between the load and the cell surface, they enabled the controlled release of particles using UV light, allowing cells to pick up, transport, and drop off cargo on demand.

This study highlights served as inspiration for using living active matter to perform mechanical work. On one hand, it demonstrates that whole microorganisms can act as microscopic carriers, and self-sustaining energy supply. On the other hand, it also underscores practical limitations: maintaining living cells, and preventing adhesion to surfaces.

Qin et al. (2007) attempted to harness the dynamics of the decomposition of previously studied hydrogen peroxide, but rather than creating a system of linear motion, they employed it in a different manner. It is a similar approach as the nanorods, that use stripes of Pt and Au, this time they use a small surface, resembling a path in one part of the rod, this configuration makes the release of oxygen bubbles in a lateral being capable of producing torque on the rod and therefore making it spin, thanks to this, they were able to create a nanorotor [82]. However, we can argue that they are not harnessing the behavior of active matter to create work, but rather making active matter behave a certain way.

Another novel demonstration of obtaining work from active matter was presented by Hiratsuka et al. (2006), who developed a microrotary motor powered by the gliding bacterium *Mycoplasma mobile* [84]. Unlike flagellated swimmers *E. coli* or *Chlamydomonas*, *M. mobile*



**Figure 4.5:** Experiments that harness bacteria motility. **Panel 1)** shows how the bacteria accumulates in the concave sections of the shuttle, finally aligning parallelly, obtained from [83]. **Panel 2** drawing of *Chlamydomonas reinhardtii*'s movement, obtained from [80]. **Panel 3) - 4)** shows an example of ratchet used in experiments, made by lithography, obtained from [15].

moves by gliding over solid surfaces at speeds of 2–5  $\mu\text{m/s}$ , using sialic proteins in the surface of the track. The authors harnessed this motility by integrating living cells into lithographically fabricated microdevices.

Their microrotary motor consisted of a circular silicon track, into which *M. mobile* cells were guided asymmetrically so that the majority moved in a unidirectional loop. A 20  $\mu\text{m}$  silicon dioxide rotor with protrusions that fit into the circular track was then docked, and cells were chemically linked to its surface via biotin–streptavidin interactions. As the bacteria glided along the track, they pulled the rotor, producing unidirectional rotation at rates of 1.5–2.6 revolutions per minute (rpm). The torque generated by individual cells was estimated to be  $2\text{--}5 \times 10^{-16}\text{ N}\cdot\text{m}$ , sufficient to overcome viscous drag at the microscale.

This work represents a successful integration of living motile cells with inorganic micromachinery, demonstrating that whole microorganisms can be harnessed to drive artificial devices.

Angelani et al. (2010) noticed how asymmetric geometry can be used to harness the ran-

domness of particles to obtain work from them. Using numerical simulations, they mimicked elongated motile bacteria, and the object to move consisted of an arrow-shaped structure with a varying number of teeth, ranging from 2 to 8. They saw that some particles get trapped between the spaces of the teeth, aligning themselves, making it possible to push the *shuttle*, and due to dynamics, they eventually get unstuck and return to swim free in the solution. The simulations were performed in 2 dimensions, where bacteria were able to push the object [83].

Beyond the use of single microorganisms as engines, researchers have also looked at how collective active matter might be used to produce work. Thampi et al. (2016) showed in simulations that dense active fluids—like bacterial suspensions or mixtures of microtubules with motor proteins—can display mesoscale turbulence that can be rectified to move micromachines [85].

In their setup, a square array of symmetric microrotors was placed inside an active nematic fluid. Although the rotors were geometrically identical, the system broke symmetry on its own: neighboring discs settled into an alternating spin pattern, rotating in opposite directions. In this way, disordered turbulent flows were turned into a regular and steady source of rotation. The extent and stability of the rotation depended on rotor size and spacing, with the best results when the separation was comparable to the natural vortex size of the active turbulence.

This study is useful here for two reasons. First, it shows that work can be obtained from active turbulence without introducing asymmetry or applying external fields. Second, it illustrates how geometry and confinement help stabilize active flows—ideas that will be relevant again in this thesis when we study colloids and ratchet systems under external driving.

A central question in active matter is how to harness the continuous energy consumption of self-propelled agents to perform useful work. Inside cells, proteins such as kinesin and dynein already fulfill this role at the nanoscale, but the prospect of exploiting entire microorganisms as microscopic engines is especially appealing. Early studies demonstrated that bacteria could be attached to synthetic objects and used to propel them forward [80, 84]. The resulting motion, however, was generally random.

A major advance came with the work of Di Leonardo et al. (2010), which served as inspiration for this thesis, showing that geometry alone can guide bacterial motion without the need for external fields [15]. In their experiments, sawtooth-shaped microgears with diameters of approximately 48  $\mu\text{m}$  were immersed in dense suspensions of motile *E. coli*. The bacteria accumulated and aligned at the concave corners of the gears, collectively exerting a torque that rotated the structures. At cell concentrations on the order of  $10^{10} \text{ mL}^{-1}$ , the gears achieved steady angular velocities of about 2 rpm. This behavior follows the mechanism described by Angelani et al. (2010), where cells become transiently trapped between the asymmetric teeth, pushing against the walls and generating directed motion [83].

Interestingly, the authors also tested different geometries. As expected, asymmetric rotors produced net rotation, while symmetric ones yielded zero average angular velocity, underscoring the importance of symmetry breaking in rectifying bacterial motion.

This result demonstrates that combining bacterial activity with asymmetric boundaries can act as a ratchet, transforming random fluctuations into directed motion. The concept recalls the Feynman ratchet thought experiment, but here it is realized in a living system, powered solely by bacterial metabolism. Such bacterial ratchets not only provide fundamental insight into nonequilibrium statistical mechanics but also suggest potential applications in microfluidics, where pumps and mixers could operate autonomously without external energy inputs.



# Chapter 5

## Magnetically Driven Colloidal Systems

We can see that biological active matter is effective at transporting or moving objects. The drawback, however, is that these systems always require a constant supply of energy. So far, there is no unlimited energy source available for this purpose. An exception are thermophoretic particles, which only need a beam of light to create a temperature gradient. In fact, some experiments have combined this principle with machine learning models, allowing particles to be guided toward a target region while reducing the impact of thermal noise [86]. The limitation, though, is that only a relatively small number of particles can be manipulated in this way, which is not enough to drive something like a rotor.

Because of this, we take a different approach. The idea is to combine active and passive matter, so that energy can be injected into the system without having to replace the entire source each time. This hybrid strategy may offer a way to overcome the limits seen in purely biological or purely synthetic setups.

This thesis focuses on paramagnetic colloids. Their key property is that the magnetic dipoles align with an external field, but once the field is removed, the dipoles lose their orientation and the material no longer shows magnetic order. The origin of this effect lies in the electronic and spin configuration of the atoms. A simple example is molecular oxygen,  $O_2$ , which has two unpaired valence electrons with the same spin. This imbalance leads to a net magnetic moment, giving rise to paramagnetism. The underlying principle is explained by Hund's rule.

By themselves, paramagnetic particles cannot be considered active matter, even in the presence of a magnetic field. Several experiments have tried to induce motion in these systems, and one promising route is through Brownian rectification. For example, Tierno (2012) studied paramagnetic colloids placed above a ferrite garnet film. The film contained permanent magnetic domains aligned along the  $x$ -axis, with alternating directions, while the colloids were subjected to a circularly precessing magnetic field in the  $y-z$  plane [18].

With these parameters, and by varying only the driving frequency, four regimes of motion were identified. At the highest frequencies, the particles entered a pinned state, meaning the colloids did not translate. Tierno also tested elliptic magnetic fields and observed that, depending on the field magnitude, the particles displayed either attractive or repulsive interactions. These behaviors arise from the dipole–dipole potential between particles, given by

$$U_{dd} = \frac{\mu}{4\pi} \left( \frac{m_i m_j}{r_{ij}^3} - \frac{3(m_i \cdot r_{ij})(m_j \cdot r_{ij})}{r_{ij}^5} \right), \quad (5.1)$$

where  $m_i$  and  $m_j$  are the magnetic moments of particles  $i$  and  $j$ , and  $r_{ij}$  is their separation vector.

A subsequent study by Straube and Tierno (2013) provided a deeper understanding of these dynamics by analyzing the role of synchronization and thermal noise [87]. Using the same ferrite garnet film with periodic magnetic domains, they investigated the motion of a single paramagnetic colloid driven by a rotating magnetic field. At low driving frequencies, the particle remained synchronized with the moving magnetic potential, resulting in constant-speed transport at the same velocity as the traveling landscape. Above a critical frequency, however, the particle lost synchronization, entering an asynchronous regime characterized by intermittent sliding and a reduced average speed.

To describe these results, Straube and Tierno proposed a simplified analytical model based on the overdamped Langevin equation, which accounted for both deterministic forces and thermal fluctuations. Importantly, their model showed excellent agreement with experiments and revealed how thermal noise smooths the sharp transition between synchronous and asynchronous regimes. This highlights the interplay between deterministic driving and stochastic forces in rectification phenomena, and demonstrates how even passive colloids can be controlled and transported through external fields when symmetry is broken.

A year later, they used the same system with a rotating magnetic field whose ellipticity could be tuned [19]. The effect of this field was to create an asymmetric traveling potential that rectified Brownian motion and transported the particles across the surface.

One of the main results was that the interaction between particles could switch from repulsive to attractive just by adjusting the ellipticity of the field. In the attractive case, particles came together into stable doublets that moved with constant velocity along the magnetic stripes. They measured the dipolar forces that caused this binding and proposed a model that matched well with the experiments.

This shows that not only single-particle motion can be controlled, but also collective effects like chain formation and cooperative transport. The fact that this can be tuned with an external field suggests possible uses in microfluidics or lab-on-chip devices, where clustering or separa-

tion of particles can be useful for transport, mixing, or sorting.

This dipole-dipole attractive and repulsive interaction between particles, is a key aspect for this thesis. More recently, Stoop et al. (2021) studied a dense monolayer of paramagnetic colloids driven above a triangular lattice of magnetic bubbles using a rotating magnetic field [88]. The external field generated a two-dimensional traveling wave ratchet that transported the particles across the substrate. While single colloids showed no preferred direction of motion, collective interactions at higher densities led to a spontaneous symmetry breaking. In this regime, the particle current locked along one of the crystallographic axes of the lattice, producing a transversal current even though the driving direction was set between two symmetry axes.

They also reported that this locking could be polarized by adding a weak bias field, which made one direction energetically favorable over the other. At intermediate densities, elongated clusters of particles formed and moved coherently, showing that dipolar interactions stabilize directional locking. At very high densities, however, the effect was lost as the colloids formed a percolating network covering the entire substrate.

This work highlights how collective effects can generate robust directional transport that does not appear at the single-particle level. It shows that by controlling density and external fields, transport in colloidal systems can be tuned or polarized, which is useful for applications such as particle sorting and microfluidic control.

A recent study by Ostinato *et al.* (2024) explored the collective dynamics of paramagnetic colloids confined between two plates separated by less than twice the particle diameter and driven by a precessing magnetic field [20]. Using numerical simulations, they demonstrated that the interplay between confinement and dipolar interactions can produce two distinct transport regimes.

When the applied precessing field was spatially isotropic, the particles did not display a net current but instead showed enhanced diffusion, with an effective diffusion coefficient up to 60 times larger than that of unforced colloids. This enhancement originated from a continuous exchange of positions between colloids near opposite walls, a motion resembling a “ceilidh dance” of dimers that bind and unbind periodically [20].

In contrast, introducing a small spatial anisotropy by tilting the precession axis ( $\delta \neq 0$ ) generated a robust bidirectional current. In this regime, colloids organized into two parallel flows moving in opposite directions, achieved by synchronized particle exchanges across the two planes. The magnitude of this current was highly tunable by varying both the driving frequency and the tilt angle, reaching maximal values when particles jumped exactly one lattice constant per field cycle. Remarkably, this bidirectional transport was robust against single-particle defects but could be disrupted by the introduction of “magnetic holes” (nonmagnetic inclusions in the ferrofluid), which acted as localized defects that broke the current pathways.

These results provide a powerful demonstration of how geometrical confinement and external field anisotropy can convert random thermal motion into ordered transport, without the need for field gradients. They highlight new opportunities for designing microfluidic devices where colloids could be directed, mixed, or sorted by simply tuning the parameters of an external homogeneous field.

## **Part III**

## **Methods**



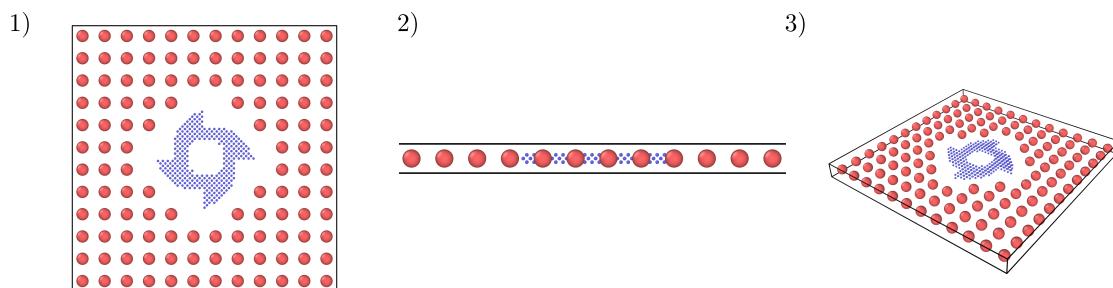
# Chapter 6

## Simulations

The system studied in this thesis consists of an ensemble of paramagnetic colloidal particles confined in a quasi-two-dimensional geometry and subjected to an externally applied precessing conic magnetic field. Each colloid is a spherical particle of radius  $r_{\text{mag}}$  suspended in a Newtonian fluid of dynamic viscosity  $\eta$ . The suspension is bounded by two parallel glass plates separated by a distance  $h$ , such that  $h \lesssim 2R$ . This strong confinement restricts particle motion primarily to two dimensions, while still allowing limited vertical displacement.

Numerical simulations provide a powerful framework to reproduce and analyze physical phenomena under controlled conditions. Unlike experiments, they allow for precise manipulation of initial parameters, systematic testing of hypotheses, and straightforward replication of results. In particular, simulations are invaluable when dealing with microscopic systems, where stochastic effects and complex interactions can make experimental observations challenging.

In this thesis, numerical simulations are employed to study the dynamics of colloidal systems at the microscale. Such systems are often dominated by thermal fluctuations and many-body interactions, making them difficult to probe experimentally without advanced imaging and



**Figure 6.1:** System overview for a non-specular ratchet

data analysis techniques. The primary computational approach used here is *molecular dynamics* (MD), which will be described in detail in the following sections. MD enables the integration of particle trajectories under the influence of deterministic and stochastic forces, providing direct access to observables such as mean-squared displacements, velocity correlations, and transport coefficients.

## 6.1 Molecular dynamics

This thesis explores the physics of the system by using molecular dynamics, where randomness enters through thermal noise. As we saw in 2.2.1, the interactions can be derived from classical mechanics. In this case, Newton's second law gives the starting point to calculate the forces acting on a single particle. In other words, at each iteration of the simulation we need to evaluate the forces that each particle experiences. Taking equation (2.4) as a starting point, and adding labels for the different interactions, we obtain:

$$m_i \ddot{\vec{x}}_i = F_i^{collision} + F_i^{drag} + \eta(t), \quad (6.1)$$

where  $m_i$  is the mass of particle  $i$ ,  $\vec{x}_i$  its position, and  $F_i^{drag}$  is the viscous force, written as  $-\lambda \dot{\vec{x}}_i$ , with  $\lambda$  the drag coefficient of the fluid. Since we are working at a scale where inertial effects are negligible, the term  $m_i \ddot{\vec{x}}_i$  can be dropped. The random force  $\eta(t)$  represents collisions with the solvent particles. In this thesis,  $\eta$  is taken as a Gaussian random force with  $\langle \eta \rangle = 0$  and correlation  $\langle \eta_i(t) \eta_j(t') \rangle = 2k_B T \lambda \delta_{i,j} \delta(t - t')$ . This form will be used for non-paramagnetic particles.

For paramagnetic particles, we need to add the contribution of dipole–dipole interactions, which gives the modified equation:

$$m_i \ddot{\vec{x}}_i = F_i^{collision} + F_i^{drag} + F_i^{dd} + \eta(t), \quad (6.2)$$

where  $F_i^{dd}$  according to [89] is described as force exerted for the dipole moment  $\vec{m}_i$  on a dipole  $\vec{m}_j$ :

$$\vec{F}_i^{dd} = \frac{3\mu_0}{4\pi r^4} \left[ (\hat{x}_{i,j} \times \vec{m}_i) \times \vec{m}_j + (\hat{x}_{i,j} \times \vec{m}_j) \times \vec{m}_i - 2\hat{x}_{i,j}(\vec{m}_i \cdot \vec{m}_j) + 5\hat{x}_{i,j}((\hat{x}_{i,j} \times \vec{m}_i) \cdot (\hat{x}_{i,j} \times \vec{m}_j)) \right], \quad (6.3)$$

where  $\hat{x}_{i,j}$  is the unitary vector of distance between dipoles. Since all magnetic dipoles are identical and aligned with the external magnetic field  $\vec{B}_{ext}$ , we can express the dipole moment as  $\vec{m} = \chi V \vec{H}_{ext} = \frac{\chi V}{\mu_0} \vec{B}_{ext}$ , where  $\chi$  is the magnetic susceptibility and  $V$  is the particle volume. Substituting  $\vec{m}_i = \vec{m}_j = \vec{m}$  and expressing in terms of the external field gives:

$$\vec{F}_{i,j}^{dd} = \frac{3\mu_0 m^2}{4\pi r^4} \left[ 2(\hat{x}_{i,j} \times \hat{B}) \times \hat{B} - 2\hat{x}_{i,j} + 5\hat{x}_{i,j}|\hat{x}_{i,j} \times \hat{B}|^2 \right], \quad (6.4)$$

where  $m = \frac{\chi V B_{\text{ext}}}{\mu_0}$ ,  $\hat{B} = \vec{B}_{\text{ext}}/B_{\text{ext}}$  is the unit vector along the external field, and  $B_{\text{ext}} = |\vec{B}_{\text{ext}}|$ .

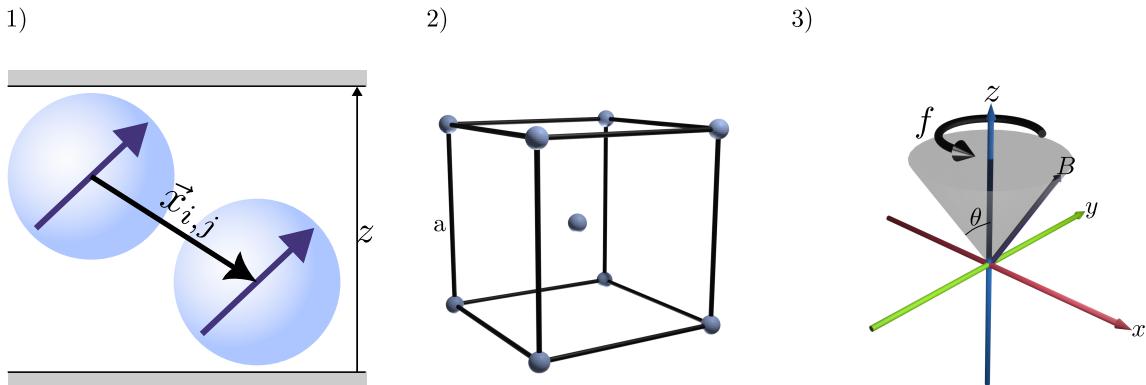
This force only applies for one particle, to obtain the total dipole interaction with all particles of the system, we should add them up, pair by pair:

$$F_i^{dd} = \sum_{i \neq j}^n F_{i,j}^{dd}. \quad (6.5)$$

For this, we need to define the external magnetic field, which it is a precessing field that forms a conical rotation of the form

$$\vec{B} = B_0[\cos \theta \hat{z} + \sin \theta \cos(2\pi ft) \hat{x} + \sin(2\pi ft) \hat{y}], \quad (6.6)$$

where  $B_0$  is the amplitude and  $f$  the frequency of rotation of the magnetic field. The frequency plays an important role in the system dynamics. Depending on how fast the field rotates, it determines whether the internal magnetic dipole of each particle can follow it or not. At low frequencies, the dipoles rotate synchronously with the field, resulting in purely attractive or repulsive interactions. At higher frequencies, however, the dipoles cannot keep up, leading to a phase delay. In this regime, particles can exchange neighbors as the field continues to rotate.



**Figure 6.2:** **Panel 1)** Shows two paramagnetic particles with a distance  $\vec{x}_{i,j}$  with the same dipole moment in a confined space in the  $z$  axis. **Panel 2)** Shows a representation of a unitary body-centered cubic lattice. **Panel 3)** Shows the precessing external magnetic field.

Let's remember that one important rule for the universe is that, one body cannot occupy the same space as other, therefore, we should model a repulsion force that simulates that behavior.

Fortunately, there is a potential called Weeks-Chandler-Andersen potential (WCA) that follow the same principle as the Lennard-Jones potential but with a cutoff [90]:

$$U_{i,j}^{WCA} = \begin{cases} 4\epsilon \left[ \left( \frac{\sigma}{r_{i,j}} \right)^{12} - \left( \frac{\sigma}{r_{i,j}} \right)^6 \right] + \epsilon & r_{i,j} \leq r_c \\ 0 & r_{i,j} \geq r_c \end{cases} \quad (6.7)$$

where  $\sigma$  is the van der Waals radius, it is the point where the energy between the two particles is zero,  $\epsilon$  is the well depth, since WCA does not have an attraction interaction, a correction factor of  $\epsilon$  is added, and  $r_c = 2^{1/6}\sigma$ . This however, gives us the energy between particles, and we need the force, then we apply:

$$F = -\nabla U, \quad (6.8)$$

getting then

$$F_{i,j}^{WCA} = \begin{cases} 48\epsilon \left[ \left( \frac{\sigma}{r_{i,j}} \right)^{12} - 0.5 \left( \frac{\sigma}{r_{i,j}} \right)^6 \right] \left[ \frac{1}{r_{i,j}} \right] & r_{i,j} \leq r_c \\ 0 & r_{i,j} \geq r_c \end{cases}. \quad (6.9)$$

and verifying the interaction between each particle, we obtain:

$$F_i^{collision} = \sum_{i \neq j}^n F_{i,j}^{WCA}. \quad (6.10)$$

We want to see how the positions of the particles evolve over time with certain initial conditions, and this equations only compare velocities, this is why we need an integration method.

## 6.2 Velocity Verlet

The Velocity Verlet algorithm is derived from the standard Verlet method by explicitly incorporating velocity terms [91, 92]. We begin with the Taylor series expansions of position.

### 6.2.1 Taylor Series Expansions

The forward Taylor expansion for position is:

$$x(t + \Delta t) = x(t) + v(t)\Delta t + \frac{1}{2}a(t)\Delta t^2 + \frac{1}{6}b(t)\Delta t^3 + O(\Delta t^4) \quad (6.11)$$

The backward Taylor expansion is:

$$x(t - \Delta t) = x(t) - v(t)\Delta t + \frac{1}{2}a(t)\Delta t^2 - \frac{1}{6}b(t)\Delta t^3 + O(\Delta t^4) \quad (6.12)$$

where  $b(t)$  represents the third derivative (jerk), and  $O(\Delta t^4)$  represents an error of magnitude  $\Delta t^4$ .

### 6.2.2 Original Verlet Algorithm

Adding equations (6.11) and (6.12) cancels the velocity and jerk terms:

$$x(t + \Delta t) + x(t - \Delta t) = 2x(t) + a(t)\Delta t^2 + O(\Delta t^4) \quad (6.13)$$

Solving for  $x(t + \Delta t)$  gives the original Verlet algorithm:

$$x(t + \Delta t) = 2x(t) - x(t - \Delta t) + a(t)\Delta t^2 + O(\Delta t^4) \quad (6.14)$$

### 6.2.3 Velocity Calculation

Subtracting equation (6.12) from (6.11) gives the velocity:

$$x(t + \Delta t) - x(t - \Delta t) = 2v(t)\Delta t + O(\Delta t^3) \quad (6.15)$$

$$v(t) = \frac{x(t + \Delta t) - x(t - \Delta t)}{2\Delta t} + O(\Delta t^2) \quad (6.16)$$

### 6.2.4 Velocity Verlet Formulation

The Velocity Verlet algorithm provides a more convenient form that explicitly tracks velocities. Starting from the forward Taylor expansion (equation 6.11):

$$x(t + \Delta t) = x(t) + v(t)\Delta t + \frac{1}{2}a(t)\Delta t^2 \quad (6.17)$$

To find the velocity at  $t + \Delta t$ , we use the average acceleration:

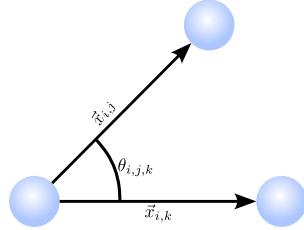
$$v(t + \Delta t) = v(t) + \frac{a(t) + a(t + \Delta t)}{2}\Delta t \quad (6.18)$$

A more numerically stable implementation uses a half-step approach:

$$v(t + \frac{1}{2}\Delta t) = v(t) + \frac{1}{2}a(t)\Delta t \quad (6.19)$$

$$a(t + \Delta t) = \frac{F(x(t + \Delta t))}{m} \quad (\text{Compute new acceleration}) \quad (6.20)$$

$$v(t + \Delta t) = v(t + \frac{1}{2}\Delta t) + \frac{1}{2}a(t + \Delta t)\Delta t \quad (6.21)$$



**Figure 6.3:** Visual representation for a harmonic angular potential.

### 6.3 Basis Vectors

The basis vectors (or lattice vectors) are the fundamental building blocks used to generate the entire crystal lattice by translation. These vectors define the geometry of the unit cell, and by repeating the unit cell across space, you form the overall lattice structure. Here, a body-centered lattice was chosen since the stability it proved to have when under thermal fluctuations.

In the body-centered lattice, the basis vectors determine the relative positions of atoms in the unit cell. These vectors are used to place atoms and generate the positions of all atoms in the simulation box.

The conventional unit cell for a BCC lattice is a cube with a lattice point at each corner and one at the body center. The vectors defining this cube are simple, orthogonal, and given by:

$$\vec{a} = a\hat{x}, \quad \vec{b} = a\hat{y}, \quad \vec{c} = a\hat{z}, \quad \vec{d} = \frac{a}{2}(1\hat{x} + 1\hat{y} + 1\hat{z}), \quad (6.22)$$

where  $a$  is the lattice constant (the side length of the cube).

There are multiple forms to model the potential energy of a bond, the easiest way is to use the harmonic potential that mimics the behavior of a ideal spring and is modeled after the Hooke's law:

$$U_{i,j}^H(\vec{x}_{i,j}) = \frac{1}{2}K(\vec{x}_{i,j} - \vec{x}_0)^2, \quad (6.23)$$

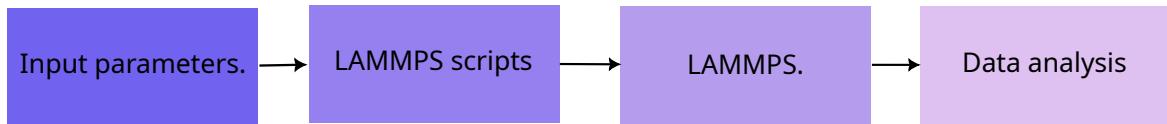
where  $K$  is the energy per squared distance,  $\vec{x}_{i,j}$  is the distance between particle  $i$ , and  $j$ , and  $x_0$  is the equilibrium distance point.

Equally, each particle has a defined angle between a triplet of particles that will help in the definition of the lattice, it is defined also with Hooke's law:

$$U_{i,j,k}^H(\theta_{i,j,k}) = \frac{1}{2}K(\theta_{i,j,k} - \theta_0)^2, \quad (6.24)$$

## 6.4 System Overview and Workflow

The simulations of this thesis were performed with an open-source software called LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) developed by Sandia National Laboratories. Its advantage is the high efficiency to run simulations in parallel, reducing the time required to perform multiple calculations [93]. We used a standard version of LAMMPS but created custom input scripts using a Python library. These scripts will automate the process of the input scripts that will tell LAMMPS everything about the parameters of our simulation, such as the size of the system, the physical conditions, and how long to run for. After the simulations, we used additional custom scripts with the help of a Python library called Pandas, to analyze the results quickly and efficiently.



**Figure 6.4:** Workflow diagram.

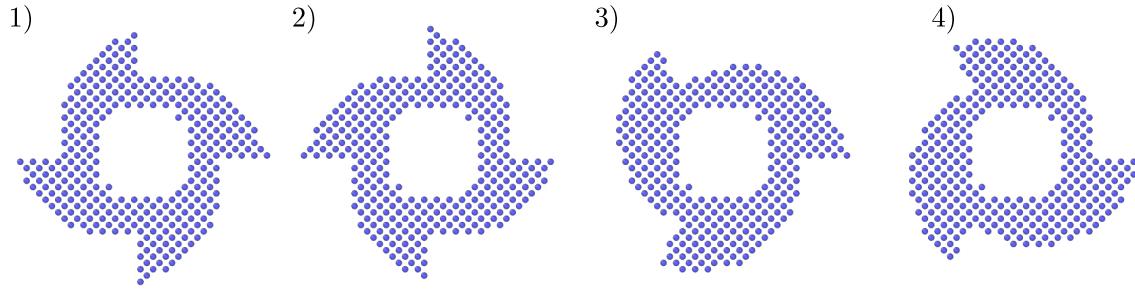
### 6.4.1 System's Physical Definition

The first parameters to be defined are the ones from the circular-ratchet geometry, since it will define the position of the paramagnetic colloids afterwards, these are the parameters that can be specified in the function:

**Table 6.1:** Parameters used for the circular ratchet in the simulation.

Parameter	Symbol	Ratchet A	Ratchet B	Units
Lattice constant	$a$	1	1	$\mu m$
Radius	$r$	8	8	$\mu m$
Sawtooth amplitude	$A$	4	4	$\mu m$
Sawtooth frequency	$N$	5	3	Dimensionless
Bond coefficient	$K_b$	0.1	0.1	$\mu N$
Density	$\rho$	1	1	$kgm^{-3}$

As shown in the table, there were 2 ratchets with only a difference in the *Sawtooth frequency*, but in reality we used a reflection of each ratchet for another pair of analysis. Once the ratchet geometry is defined, then we can define then the remaining of the system, which remained constant



**Figure 6.5:** Ratchet geometry used in the simulations. **Panel 1)** shows 4-spikes ratchet.**Panel 2)** shows the same ratchet with a  $180^\circ$  specular rotation. **Panel 3) - 4)** Shows the same characterisites with a 3-spikes ratchet.

for the 2 ratchets. Starting with the simulation box, that is a rectangle box of periodic boundary conditions in axis  $x$ , and  $y$ ,and finite boundary conditions modeled with the a WCA potential:

**Table 6.2:** Parameters used for the box of the simulation.

Axis	lo	hi	Units
$x$	-27	27	$\mu m$
$y$	-27	27	$\mu m$
$z$	-2	2	$\mu m$

Where  $lo$  represent the lower boundary, an  $hi$  the upper boundary.

Finally, for the paramagnetic particles, and since they deppend on the magnetci field, we included the parameters of this one too

**Table 6.3:** Parameters used for the paramagnetic particles.

Parameter	Symbol	Value	Units
Radius	$r_{mag}$	1.25	$\mu m$
Susceptibility	$\chi$	0.4	Dimensionless
Field angle	$\theta$	27	$^\circ$
Frequency	$f$	[0 - 10]	Hz

With all this values, we can run simulations for a period of  $50 \times 10^6 \mu s$ , with a timestep of 10  $\mu s$  which corresponds to a total real time of 500s (8.333min). Since these systems are of random nature, it is recommended to perform multiple simulations in order to be able to obtain statistics, therefore we ran it 10 different times for each frequency.

### 6.4.2 Data Analysis

When finishing a simulation, LAMMPS will give a text data file with values we chose to obtain. In this case we were interested in the position of the particles to be able to deduce some information, being the angular velocity the more interesting one. The system consists of multiple particles, each one of them having a different angular velocity due to bond not being strong enough to maintain particles static, therefore we need to obtain an average velocity for the entirety of the particles. What we know, is that every particle shares the same center of mass that is calculated as follows:

$$(x_{\text{COM}}, y_{\text{COM}}) = \frac{\sum_{i=1}^n m_i * r_i}{\sum_{i=1}^n m_i}. \quad (6.25)$$

Being  $m_i$  the mass of the particle  $i$ , and  $r_i$  the position of the particle respect a frame of reference. The best way to calculate the angular velocity is by using polar coordinates:

$$r_i = \sqrt{(x - x_{\text{COM}})^2 + (y - y_{\text{COM}})^2}, \quad (6.26)$$

$$\theta_i = \arctan \frac{y - y_{\text{COM}}}{x - x_{\text{COM}}}. \quad (6.27)$$

Once obtained the center of mass and the polar coordinates of each particle, then we can calculate the angular velocity of each particle for each timestep of the simulation:

$$\omega_i = \frac{\Delta\theta_i}{\Delta t}, \quad (6.28)$$

then obtaining an average angular velocity of all particles.



# **Part IV**

# **Results**



# Chapter 7

## Results

To obtain some statistics from 230 simulations per ratchet, we decided to obtain the mean angular velocity over the different seeds of each frequency, and to validate the accuracy of each result, we used the error over the mean [94]:

$$\sigma_{\bar{x}} = \frac{\sigma}{\sqrt{n}}. \quad (7.1)$$

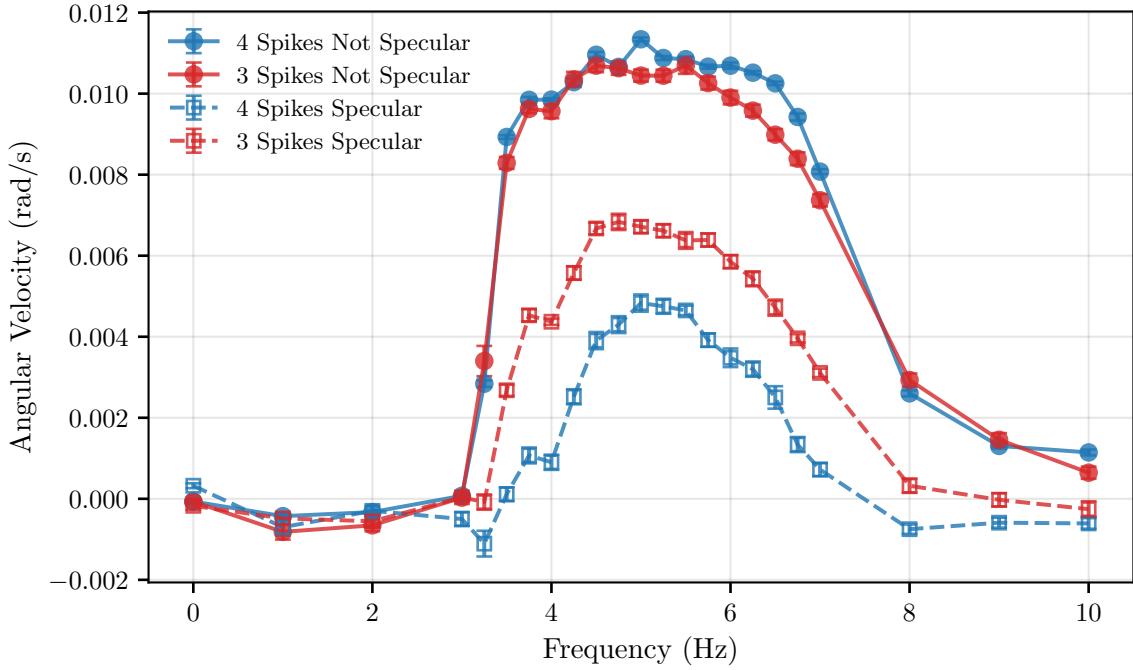
Figure 7.1 summarizes the main result of this work, showing how the average angular velocity of the system changes with the frequency of the rotating magnetic field. At low frequencies (0–3 Hz), the internal dipoles of the paramagnetic colloids can align and rotate in phase with the external field, producing almost no net rotation of the ratchet. In this regime, the particles are merely diffusive, which aligns with theoretical expectations.

As the frequency increases, the dipoles begin to experience a delay relative to the field rotation. This phase lag reduces the alignment efficiency, and the system gradually loses synchronization, reaching a peak mean angular velocity at 5 Hz. Beyond this critical frequency, the particles no longer move by exchanging neighbors but instead begin to experience enhanced diffusion.

We also observe that the geometry of the ratchet does not play a significant role in the speed; however, it has a non-negligible impact when a 180° specular rotation is performed.

This behavior demonstrates how the balance between magnetic coupling and field rotation controls the system’s dynamics. The critical frequency marks the transition out of the ratchet-like regime, beyond which the system becomes dominated by thermal fluctuations and phase delay.

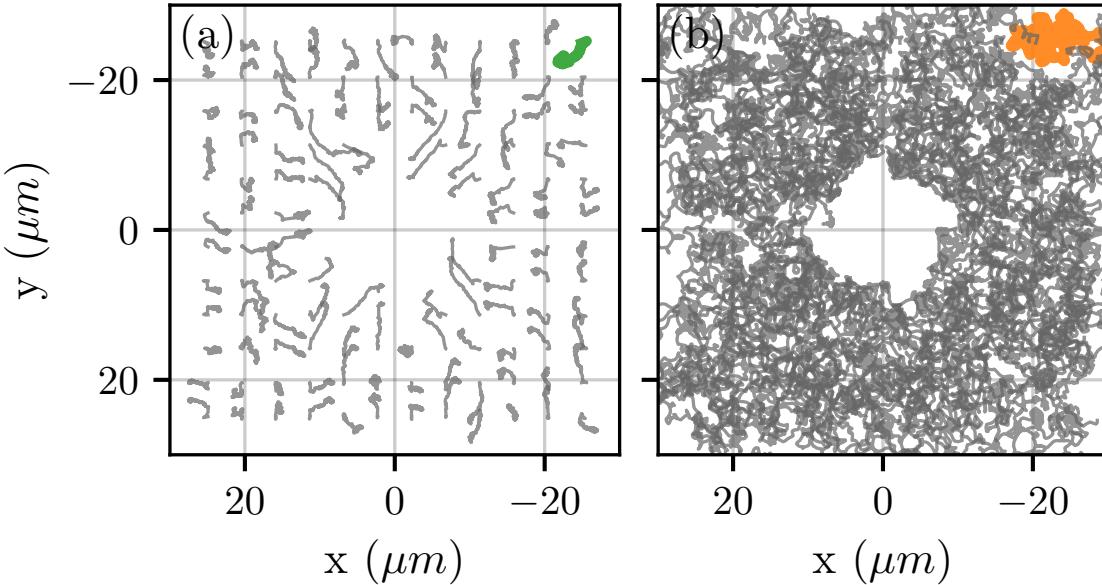
Figure 7.2 shows the particle trajectories for two representative cases: 0 Hz and 5 Hz. When no field rotation is applied (0 Hz), the particles move randomly due to thermal noise, producing isotropic diffusion with no net direction, although it is evident that the particles that are closer



**Figure 7.1:** Average angular velocity of the paramagnetic colloidal cluster as a function of the rotating magnetic field frequency.

to the ratchet feels an attraction towards it whereas the further ones reamin almost fixed in one place not experiencing the same displacement. This is an interesting beavior because there is no explicit potential that has an attractive effect between each particle. At 5 Hz, however, the trajectories reveal a rotational pattern, indicating that the dipoles are not synchronized with the external field and move collectively. This difference confirms that the rotation frequency of the magnetic field directly controls the transition from random to directed motion, as also reflected in the angular velocity results shown in Fig. 7.1, it is highlighted the trajectory of one single particle to be able to see the difference in the behavior it has each driving frequency. For 0 Hz, the trajectory seems to be quasi-static, nevertheless for 5 Hz it is evident the chaotic movement the particles have.

Since the angular velocity has very strong fluctuations, a graph over the time will not give us important visual guides wether to determine the properties. Therefore we used a type of convolution known as moving average to obtain a smoother plot. This type of mean focus on a group of values to then forget them to focus on another new group. According to [95] a two and one sided averages are given respectively by:



**Figure 7.2:** Trajectories of the particles of one simulation during the simulation, from 0 - 10 s, for (a) 0 Hz and (b) 5 Hz.

$$z_t = \frac{1}{2k+1} \sum_{j=-k}^k y_{t+j}, \quad t = k+1, k+2, \dots, n-k, \quad (7.2)$$

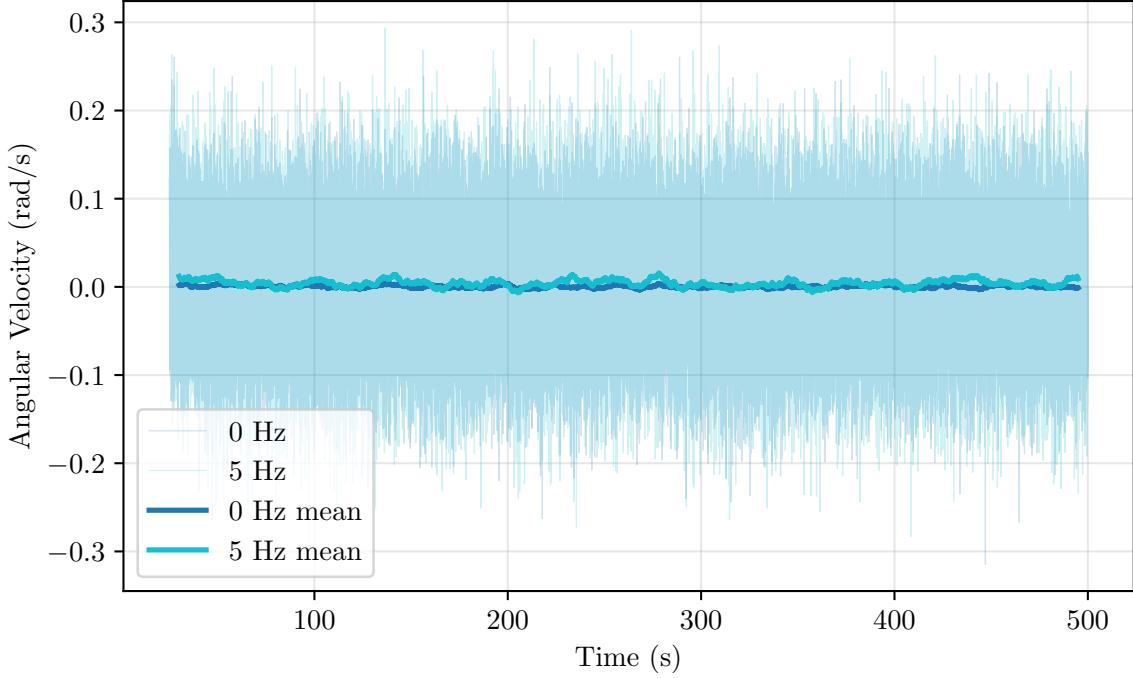
$$z_t = \frac{1}{k+1} \sum_{j=0}^k y_{t-j}, \quad t = k+1, k+2, \dots, n. \quad (7.3)$$

This, in fact, is a low-pass filter, perfect for the high peak fluctuations.

Figure 7.3 presents the time evolution of the angular velocity. At 0 Hz, the system exhibits only random fluctuations caused by thermal noise, with an average angular velocity close to zero. In contrast, at 5 Hz, the angular velocity remains consistently positive over time, despite instantaneous fluctuations. The rolling mean highlights this difference, showing a net rotational trend, in certain points, that reflects the impact the collective rotation of colloids have in the rotation of the ratchet.

This comparison illustrates how applying a conic rotating magnetic field transforms purely diffusive motion into coherent rotation, consistent with the averaged results in Fig. 7.1.

Due to the inherent variability of stochastic processes, a large amount of data is required to obtain reliable statistics. Figure 7.4 shows the angular velocity histograms for 0 Hz and 5 Hz.



**Figure 7.3:** Angular velocity of the ratchet as a function of time for a single simulation at 0 Hz and 5 Hz. The shaded regions correspond to the raw data, and the solid lines show the rolling mean.

Interestingly enough, the data showed a gaussian distribution and just as we did with the moving average, we used a Gaussian Kernel Density Estimation (KDE) to smooth out the histogram [96].

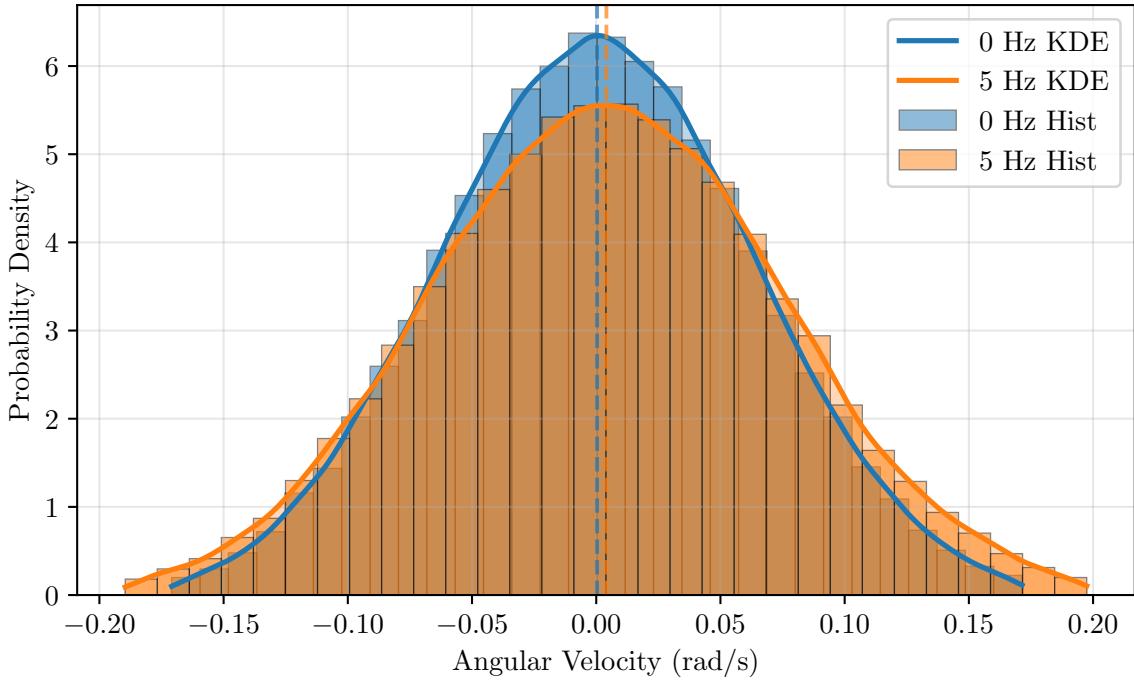
$$\hat{p}_n = \frac{1}{nh^d} \sum_{i=1}^n K\left(\frac{x - X_i}{h}\right) \quad (7.4)$$

$$K(x) = \frac{\exp(-||x||^2/2)}{v_{1,2}}, \quad v_{1,2} = \int \exp(-||x||^2/2) dx. \quad (7.5)$$

The center, which represents the mean, of the 0 Hz distribution lies almost exactly at 0 rad/s, while the 5 Hz distribution is skewed to the left, indicating a high probability of a positive net rotation and backing up the results of Figure 7.3.

Even though angular velocity gives us a big picture of how the ratchet will change over time, it is important to see the actual rotation the ratchet had in the total of 500 s.

Figure 7.5 shows the angular displacement of a single ratchet particle over the entire simulation. At 0 Hz, the particle shows an initial displacement but remains largely constant over time,



**Figure 7.4:** Histogram of angular velocity of the ratchet for a single simulation at 0 Hz and 5 Hz.

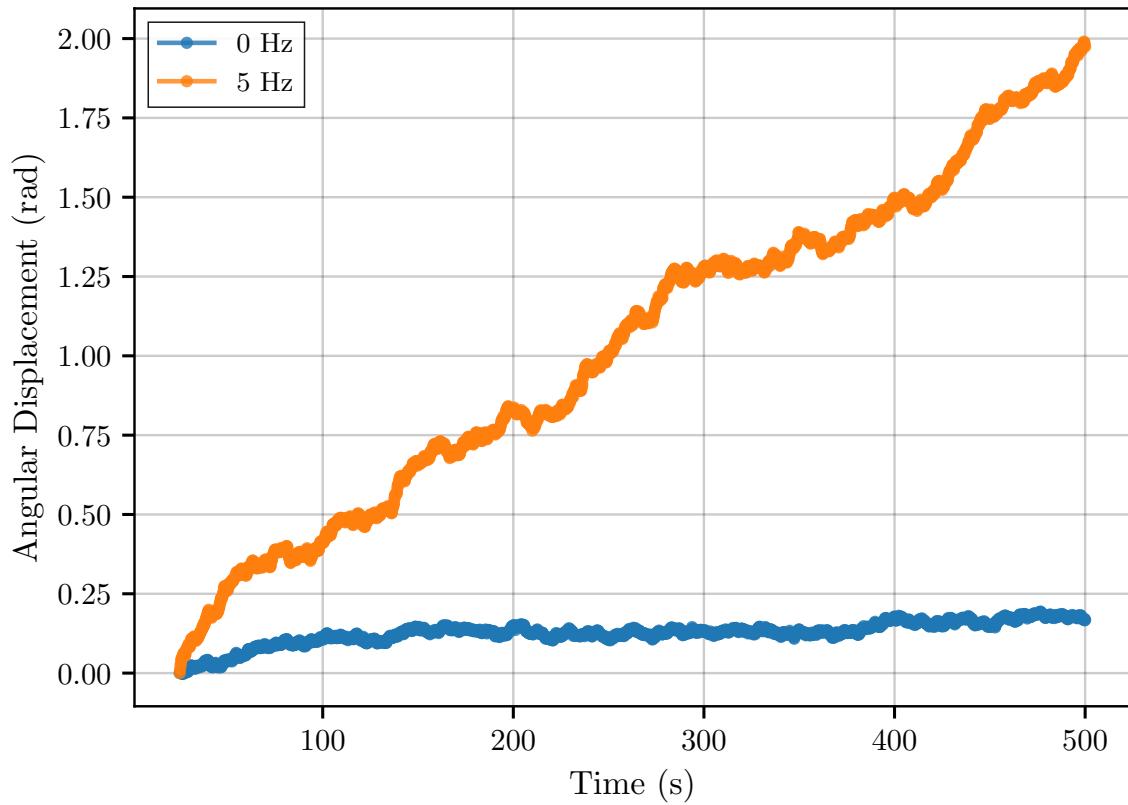
experiencing only thermal fluctuations. This initial displacement can be due to the initial interaction of the closer colloids, which move close to the walls of the ratchet and probably moving or rotating the ratchet a certain, but negligible amount, however, the remaining section is the tendency of not moving for a long period of time. In contrast, at 5 Hz, the particle exhibits a net displacement that resembles a diagonal line.

To give meaning to the plot, we can obtain the arc length of a circle, this is assuming this as an ideal trajectory for the ratchet, therefore we use the following equation:

$$s = r\theta, \quad (7.6)$$

where  $s$  is the arc length,  $r$  is the radius of our ratchet and  $\theta$  is the angle formed from the particle to the initial position. In this case we can see that its final angular position is  $\theta \approx 2\text{rad}$ , and to translate it into a more digestible information we use Eq. (7.6) obtaining that the particle total distance traveled was  $s \approx 16\mu\text{m}$ .

In the total simulation, the ratchet experienced a little less than half rotation but more than a quarter, but according to Purcell [1], at those regimes movement not necessarily has to be much. Nevertheless, this provides clear evidence of the frequency's dramatic effect on ratchet rotation. This aligns with the theoretical principle that work cannot be extracted from thermal fluctua-



**Figure 7.5:** Angular displacement of a particle of one simulation at 0 Hz and 5 Hz.

tions alone. However, we have identified a range of frequencies where colloidal interactions are sufficient to drive ratchet rotation.

## **Part V**

### **Conclusions**



# Chapter 8

## Conclusions

We have seen how motion at small scales becomes difficult due to the increase in the relative viscosity of fluids, which suppresses inertia and makes displacement dependent on shape or available degrees of freedom. Random forces, known as thermal fluctuations, also play an important role by constantly disturbing the motion of particles. Nevertheless, both theory and experiments have shown that even passive particles can achieve rectified motion when subjected to specific asymmetric conditions. In this thesis, we focused on ratchet effects, particularly those observed under optical tweezers.

We also discussed advances in artificial active particles, while emphasizing natural systems. These biological microswimmers demonstrate how energy can be converted into motion and even into useful work, giving rise to micromachines capable of transporting objects or generating rotation through chemical or biological activity. However, these systems face practical limitations: they are prone to biological degradation and require a continuous source of energy to remain active.

For this reason, we turned back to passive systems under external stress, focusing on spherical paramagnetic colloids driven by an external magnetic field. Experimental studies have already demonstrated that it is possible to rectify the motion of such particles, typically using ferrite garnet films to generate the required asymmetry. Yet, there also exist examples where directed motion is achieved without these substrates, relying only on a conical magnetic field.

In this thesis, we explored the effects of a conical external magnetic field on paramagnetic spherical colloids suspended in water and confined geometry. The system was studied using Brownian and molecular dynamics simulations. We analyzed physical quantities such as angular displacement and angular velocity, as they are key indicators of motion rectification.

Our analysis suggests that in the frequency range of 3.25–8 Hz there is a noticeable increase in angular velocity, which remains roughly constant—though with some fluctuations—between

3.75 and 7.75 Hz. This indicates partial rectification of motion. Although the effect is not strong enough to produce complete rotations within short timescales, it opens a new line of research to enhance the efficiency of this type of system. The same behavior was observed for all four ratchet configurations studied. Interestingly, when the ratchet geometry was rotated by 180°, the overall direction of rotation remained unchanged, even though the ratchet walls were mirrored. This raises an open question about whether the rotation can be controlled through geometry or if it depends entirely on the external magnetic field.

To ensure the accuracy of these results, we performed additional analyses on individual datasets using a moving mean filter, and histogram for the lowest (0 Hz) and highest (5 Hz) frequencies. These results confirmed the overall behavior observed in the averaged data and validated our main findings.

In summary, we explored how it is possible to obtain work from passive environments when induced in asymmetric potentials in non-symmetric objects. This thesis opens to discussion about how other parameters of the geometry of the ratchet can effectively affect the rotation of it, such as the radius, *wall length*, a lower or bigger amount of *spikes*, a bigger amount of colloids, different colloids radius.

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# Curriculum Vitae

*Yeray Cruz Ruiz* was born in Tlalnepantla, Estado de México, México. He received a Bachelor of Science degree in Mechatronics (2021) from Tecnológico de Monterrey, Campus Monterrey, México, where he is currently a full-time master's student in Nanotechnology, focusing on computational studies of soft matter systems out of thermodynamic equilibrium. His research interests include Soft Matter Physics, Colloidal Models, Passive Matter, and Active Matter, and Computational Physics.