Self-assembled rotating colloids in an active medium

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Abstract: This work investigates the behavior of passive colloidal particles immersed in a chiral active fluid composed of ferromagnetic rotors subjected to a rotating magnetic field. Using numerical simulations, we study how the translational diffusion of passive particles is influenced by the spinning frequency of rotors, the vertical height above a no-slip boundary, and the emergent structural organization of the system.

Our results show that the diffusion coefficient D of passive particles depends strongly on both the spinning frequency Λ and the height h: it increases linearly at short distances ($h = 1$), saturates at intermediate heights ($h = 2$), and exhibits a non-monotonic trend at larger separations ($h = 5$). We also analyze the radial distribution function to estimate the average cluster size ℓ, and find a strong linear correlation between ℓ and D, suggesting that collective organization enhances transport.
Keywords: active matter, non-equilibrium systems, clusters, rotating colloids, simulations
SDGs: This work is related to 4 and 9

I. INTRODUCTION

The study of self-assembly in condensed matter systems is a topic of increasing relevance due to its wide-ranging applications in biology, chemistry, materials science, and beyond. These phenomena often arise in equilibrium systems, where matter organizes into specific patterns or phases. However, when systems are driven out of equilibrium through external energy input or applied forces, novel structures can emerge—structures that cannot form under equilibrium conditions and are of significant scientific interest.

Active matter systems, composed of self-driven particles that continuously consume energy to generate forces, stresses, or motion, exemplify such non-equilibrium systems. Among them, a particularly interesting class—and the focus of this study—are spinning particles, or rotors. These particles or colloids do not exhibit translational self-propulsion but interact with their surroundings via hydrodynamic flows resulting from their rotational motion. As a consequence, these systems break both parity and time-reversal symmetry, giving rise to rich collective behaviors.

Recent experiments [1] have demonstrated that ferromagnetic colloids subjected to a rotating magnetic field can spontaneously form rotating clusters. Moreover, the interplay between dipolar magnetic interactions and hydrodynamic flows plays a critical role in the dynamics. Notably, the size and number of these clusters—and even whether they form at all—depend strongly on the spinning frequency.

The motivation of this work is to simulate and investigate the motion of passive particles, which do not interact with the external magnetic field, within these active matter environments. In particular, we aim to characterize their long-time behavior, where diffusive dynamics are expected. Specifically, we analyze how the translational diffusion coefficient depends on the rotation frequency of the active particles, and how it relates to the hydrodynamic friction, cluster size, and particle interactions.

II. THEORETICAL BACKGROUND

Active matter systems are composed of individual units that consume energy and generate motion or mechanical stress. A particular class of such systems consists of spinning particles, or rotors, which do not exhibit translational self-propulsion but interact via hydrodynamic interactions (HIs). These systems break both time-reversal and parity symmetry, and at large scales can be described as chiral active fluids.

In this study, we consider a chiral active fluid composed of ferromagnetic particles subjected to a rotating in-plane magnetic field. The torque experienced by the particles is given by:

$$\tau_m = |\vec{m} \times \vec{B}| = mB \sin\phi, \qquad (1)$$

where $\vec{m}$ and $\vec{B}$ are the magnetic moment and field, respectively, and ϕ is the phase lag between them. In the overdamped regime, the torque balance is:

$$\tau_m + \tau_v = 0, \quad \text{with} \quad \tau_v = -\zeta_r \dot{\beta}, \quad \beta = \omega t - \phi, \qquad (2)$$

where τ_v is the viscous torque and ζ_r is the rotational friction coefficient.

Each rotor generates an azimuthal flow field that decays as:

$$\mathbf{u} = \frac{\tau_m}{8\pi\eta r^2}\, \hat{z} \times \hat{r}, \qquad (3)$$

where η is the viscosity of the fluid and r is the distance from the rotor. This flow induces long-range hydrodynamic effects, which are key to cluster formation.

In addition to hydrodynamic interactions, the particles also interact magnetically through a time-averaged dipolar attraction:

$$\langle U_m \rangle = -\frac{\mu_0 m^2}{8\pi r^3}, \tag{4}$$

which is independent of the field frequency.

We model the collective dynamics by treating each particle as a point-like object subject to three types of interactions:

- Constant spinning at angular velocity ω
- Pairwise Lennard-Jones interactions:

  $$V_{LJ}(r) = 4\varepsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right],$$

  where $\sigma/2 = a_0$ is the effective radius of the particles and r is the distance between two different colloids.
- Hydrodynamic interactions via the Blake tensor, which incorporates wall-induced effects using image systems to satisfy the no-slip boundary condition.

The overdamped equation of motion for each particle is:

$$\gamma\, \dot{\mathbf{r}}_i(t) = \mathbf{u}(\mathbf{r}_i(t)) - \sum_{j \neq i} \nabla_i V(r_{ij}) \tag{5}$$

with $\gamma = 3\pi\eta\sigma$ the translational friction coefficient. Hydrodynamic interactions are accounted for through $\mathbf{u}(\mathbf{r}_i(t))$, the flow field at $\mathbf{r}_i$ due to all other particles. This flow can be decomposed into two components: one from force singularities (Stokeslets), $\mathbf{u}_S$, and another from torque singularities (Rotlets), $\mathbf{u}_R$:

$$\mathbf{u} = \mathbf{u}_S + \mathbf{u}_R.$$

These two terms are described in more detail in [2].

Additionally, we consider a different class of colloids, referred to as passive particles, which do not experience magnetic interactions and do not rotate. These particles are influenced by the flow field generated by active rotors and, in turn, disturb the fluid around them.

At short timescales, the mean square displacement (MSD) of passive particles is expected to grow quadratically:

$$\text{MSD}(t) \propto v^2 t^2.$$

However, in the steady state, passive particles undergo diffusive motion, characterized by:

$$\langle |\vec{r}(t) - \vec{r}_0|^2 \rangle = 4Dt \quad \text{(in 2D)} \tag{6}$$

where D is the translational diffusion coefficient and $\langle |\vec{r}(t) - \vec{r}_0|^2 \rangle$ is the mean square displacement. This diffusive behavior at long times can be used to extract the effective translational diffusion coefficient of passive particles immersed in active chiral environments.

III. METHODOLOGY

The evolution of the system was simulated following Eq. (5), where active particles attract each other through the force derived from the Lennard-Jones potential, $F_{ij} = -\nabla_i V_{LJ}(r_{ij})$. However, the dominant contribution to the dynamics arises from the flow field $\mathbf{u}(\mathbf{r}_i(t))$ generated by the continuous spinning of the active particles.

Passive particles, on the other hand, do not interact via the Lennard-Jones potential. Instead, their interactions are governed by the Weeks–Chandler–Andersen (WCA) potential:

$$V_{\text{WCA}}(r) = \begin{cases} V_{LJ}(r) + \varepsilon & r \leq 2^{1/6}\sigma \\ 0 & r > 2^{1/6}\sigma \end{cases} \tag{7}$$

This corresponds to a truncated and shifted Lennard-Jones potential that retains only the repulsive part. It ensures that particles repel each other when the distance between them is less than $r_m = 2^{1/6}\sigma$, the point where V_{LJ} changes from attractive to repulsive.

Moreover, the motion of passive particles is influenced by the flow field $\mathbf{u}(\mathbf{r}_i(t))$ generated by the surrounding rotors. Since passive particles do not spin, their hydrodynamic contribution is limited solely to the Stokeslet component, $\mathbf{u}_S$.

Simulations were performed for various configurations, varying parameters such as the particles height (distance from the wall) and spinning frequency. However, all simulations shared the same initial configuration: a square grid with small random displacements in particle positions and zero initial velocity.

The mean square displacement (MSD) of the passive colloids was calculated considering periodic boundary conditions and averaging over time intervals Δt between different configurations, defined as $r_i(t) = r_i(t_0 + \Delta t)$, where $r_i(t_0)$ are the particle positions at the initial time. To improve statistical accuracy, MSD was computed by shifting the initial time t_0 forward at each step. As a consequence, fewer data points are available for large Δt, which may lead to deviations from the expected diffusive behavior. Finally, the result was averaged over all passive particles.

To study the dependence of the translational diffusion coefficient D on cluster size, we also computed the radial distribution function (RDF) to estimate the mean cluster radius:

$$g(r) = \frac{1}{\rho N} \left\langle \sum_{i=1}^{N} \sum_{j \neq i} \delta(r - |r_i - r_j|) \right\rangle \Big/ (2\pi r\, \delta r), \tag{8}$$

where $g(r)$ is the RDF, ρ is the particle density, N is the number of particles, and $2\pi r\, \delta r$ is the area of the thin ring used to count how many particles are at a distance close to r.

Units: All results are expressed in reduced units, where length is set by the particle radius $a_0 = 1$, energy by $\varepsilon = 1$, and friction by $\gamma = 3$. The corresponding time unit is $\tau = \gamma a_0^2/\varepsilon = 3$.

IV. RESULTS

In this section, we present and analyze the results obtained from the simulations. We explore how the system behaves under different parameter configurations, including the spatial distribution of particles and the corresponding mean square displacement (MSD) curves. From these, we extract the translational diffusion coefficient. Additionally, we compute the radial distribution function (RDF) for various cases to estimate the average cluster size and investigate its correlation with the diffusion behavior.

To better understand the structure of the system under different driving conditions, Fig. 1 shows snapshots of the stationary states for four different values of the dimensionless spinning frequency Λ, while keeping the height fixed.

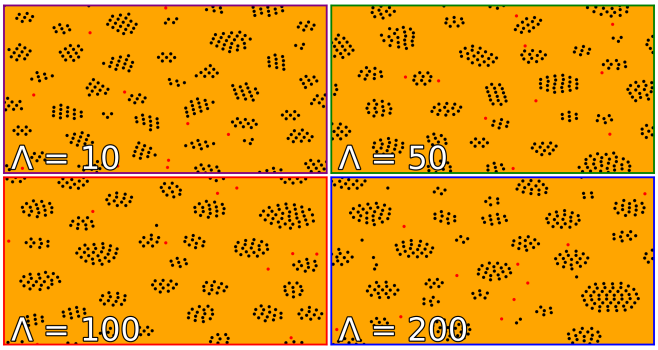

FIG. 1: Stationary particle configurations for different values of the dimensionless spinning frequency $\Lambda = \omega a_0^2 \gamma / \varepsilon$, with fixed height $h = 1$. The simulation parameters are $a_0 = 1$, $\varepsilon = 1$, and $\gamma = 3$, expressed in rescaled units based on the particle radius, interaction strength, and friction coefficient, respectively. Although values are given in reduced units, physical scales are consistent with those used in [1], where particle sizes are of the order of micrometers. The total number of particles is $N = 400$, including 390 active rotors (black) and 10 passive colloids (red). The global density is $\rho = 0.05$.

From Fig. 1, we observe that the number and size of clusters depend on the spinning frequency Λ. For a fixed height $h = 1$, higher frequencies lead to fewer but larger and more compact clusters, while lower frequencies result in a greater number of smaller clusters.

Interestingly, this trend differs from the experimental observations reported in [1], where larger clusters were found at lower frequencies. This discrepancy could be attributed to differences in system parameters such as particle height, density, or the strength of the ferromagnetic interactions. Further investigation would be needed to determine the dominant factor responsible for this deviation.

We studied the mean square displacement (MSD) of passive particles as a function of time under different system configurations. Fig. 2 shows a representative example of the MSD behavior as a function of the time lag Δt between two configurations.

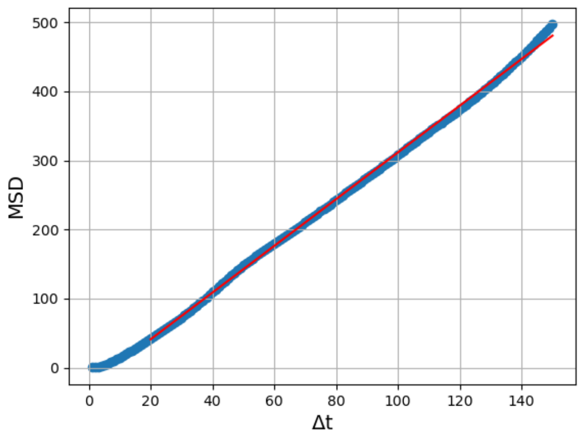

FIG. 2: Mean square displacement (blue) of passive particles as a function of the time lag Δt for $h = 2$ and $\Lambda = 10$. The red line shows a linear regression performed for $\Delta t \geq 20$. The resulting fit is $y = (3.383 \pm 0.010)x - (26.8 \pm 0.9)$, with $R^2 = 0.9990$.

As shown in Fig. 2, two distinct regimes can be identified. For short time lags ($0 \leq \Delta t \leq 20$), the MSD exhibits a quadratic-like increase, characteristic of a ballistic regime dominated by the instantaneous response to the surrounding flow. At longer times ($\Delta t \geq 20$), the MSD evolves linearly with time, indicating the onset of diffusive behavior. The slope of the linear regime allows us to extract the translational diffusion coefficient D.

By performing simulations under different conditions, we were able to study the dependence of the diffusion coefficient on several parameters. From Eq. (6), the coefficient D can be extracted directly from the slope m of the linear MSD fit via:

$$D = \frac{m}{4}$$

Fig. 3 shows the translational diffusion coefficient D of passive colloids as a function of the dimensionless spinning frequency Λ, for three different heights: $h = 1$, 2, and 5.

The trend for $h = 1$ is clearly linear, with D increasing with frequency. This suggests that the closer the passive particles are to the rotors and the boundary, the more strongly they are affected by hydrodynamic flows, which are enhanced at higher spinning rates.

For $h = 2$, the diffusion coefficient is very low at the smallest spinning frequency but increases sharply with a slight increase in Λ. This initial jump suggests that rotor activity is initially too weak to generate flows capable of significantly mobilizing the passive particles. After this threshold, however, D reaches a plateau and remains approximately constant at higher frequencies. This behavior indicates the presence of a saturation regime, where

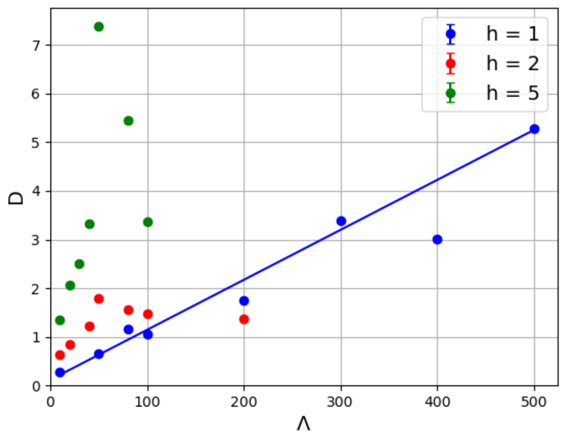

FIG. 3: Translational diffusion coefficient D of passive colloids as a function of the spinning frequency Λ, for three different heights: $h = 1$ (blue), $h = 2$ (red), and $h = 5$ (green). Error bars are included but barely visible due to their small size. A linear fit was applied to the $h = 1$ data (excluding the penultimate point), yielding $y = (0.0103 \pm 0.0005)x + (0.12 \pm 0.13)$ with $R^2 = 0.990$.

further increases in rotor spinning frequency do not enhance passive diffusion. The flow structures generated appear to be sufficiently strong above this threshold to sustain a steady level of mobility, regardless of additional increases in Λ. However, further data at higher frequencies would be needed to confirm this claim.

For $h = 5$, the diffusion coefficient also exhibits a sharp increase at low frequencies, similar to the behavior observed at $h = 2$. However, beyond this initial jump, D decreases significantly as the spinning frequency Λ increases. This non-monotonic behavior suggests that passive particle mobility is maximized at intermediate rotor activity and becomes suppressed at higher frequencies. A possible interpretation is that at low frequencies, the hydrodynamic flows generated by the rotors are more extended and coherent, effectively transporting passive particles. As the frequency increases, these flow structures may become more localized or disordered, reducing their ability to drive long-range transport and thereby lowering the diffusion of passive colloids.

In both cases, the steep jump suggests the presence of a threshold spinning frequency necessary to activate effective hydrodynamic coupling between the rotors and passive particles.

Overall, the data suggest that the effect of rotor activity on passive particle mobility is height-dependent, and reveal the existence of distinct dynamical regimes depending on both parameters.

To quantify the structural organization of the rotors, we computed the radial distribution function (RDF) for different heights and spinning frequencies. Fig. 4 shows the RDF for a fixed height and frequency. From this function, we extract the average cluster size $\ell = L/a_0$ (with $a_0 = 1\ \mu$m) as the position of the last significant peak before $g(r)$ stabilizes at 1 — beyond this point, particles are considered no longer part of the same cluster.

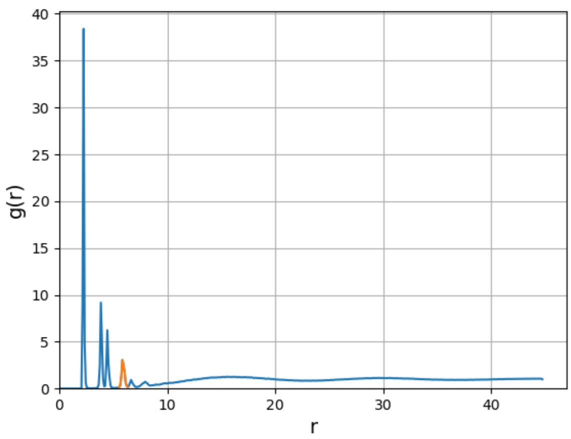

FIG. 4: Radial distribution function at $h = 1$ and $\Lambda = 10$. The peak used to estimate ℓ is highlighted in orange. The extracted average cluster size is $\ell = 5.85 \pm 0.1$.

Fig. 5 shows the estimated cluster size ℓ as a function of spinning frequency Λ for three different heights.

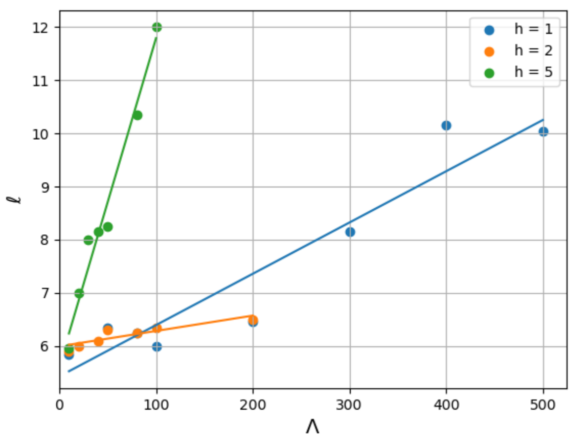

FIG. 5: Average cluster size ℓ as a function of the dimensionless spinning frequency Λ, for three different heights: $h = 1$ (blue), $h = 2$ (orange), and $h = 5$ (green). Linear regressions yield: $y_1 = (0.0096 \pm 0.0013)x + (5.4 \pm 0.3)$, $R^2 = 0.91$; $y_2 = (0.0029 \pm 0.0007)x + (5.99 \pm 0.06)$, $R^2 = 0.8$; and $y_5 = (0.062 \pm 0.005)x + (5.6 \pm 0.3)$, $R^2 = 0.97$.

From Fig. 5, we observe distinct trends depending on height. For $h = 1$, the average cluster size ℓ increases gradually with frequency, indicating that higher rotor activity promotes the formation of larger clusters. At $h = 2$, ℓ remains nearly constant, suggesting a saturation regime in which increasing frequency no longer enhances clustering. In contrast, for $h = 5$, a much steeper dependence is observed, with ℓ increasing rapidly even with small variations in Λ.

These results confirm that the spatial organization of active rotors is highly sensitive to both spinning frequency and vertical position, and provide a structural basis for investigating how these factors influence passive particle diffusion.

Finally, we analyze the relationship between the average cluster size ℓ and the translational diffusion coefficient D. The aim is to determine whether the degree of structural organization influences the diffusive motion of passive colloids, which is relevant for understanding how collective active dynamics affect transport properties.

Fig. 6 shows the measured values of D as a function of the mean cluster size ℓ. A linear regression was performed on the data points shown in blue, excluding outliers (in red) that deviate significantly from the general trend. The resulting fit is:

$$D = (1.04 \pm 0.06)\,\ell - (5.3 \pm 0.4), \quad R^2 = 0.95.$$

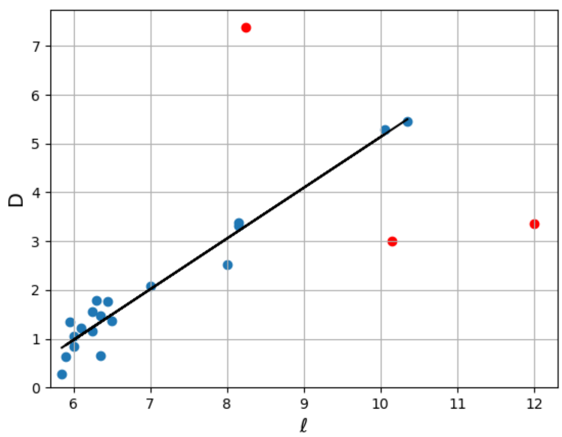

FIG. 6: Translational diffusion coefficient D as a function of the average cluster size ℓ. A linear regression (black line) was performed on the blue points, excluding red-marked outliers.

Overall, the data reveal a strong linear correlation between cluster size and diffusion: the translational diffusion coefficient increases proportionally with ℓ. This suggests that larger clusters facilitate enhanced transport of passive particles, possibly due to cooperative hydrodynamic effects or the modification of the local flow field in more structured environments.

V. CONCLUSIONS

The main conclusions drawn from this work are:

- Passive particles immersed in a chiral active fluid exhibit diffusive behavior at long timescales, which can be quantified through the mean square displacement (MSD).
- The translational diffusion coefficient D strongly depends on the vertical distance h:
  - At $h = 1$, D increases linearly with the spinning frequency Λ, indicating strong hydrodynamic coupling.
  - At $h = 2$, D increases sharply at low frequencies and then saturates, suggesting the emergence of a threshold-driven regime.
  - At $h = 5$, D shows a non-monotonic behavior: it peaks at intermediate Λ and decreases at high frequencies.
- The structure of the rotor system changes with frequency: cluster size ℓ increases with Λ for $h = 1$ and $h = 5$, while it remains nearly constant at $h = 2$.
- There exists a strong linear correlation between the average cluster size ℓ and the diffusion coefficient D, indicating that more organized or larger rotor clusters enhance passive transport.

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I would like to sincerely thank my advisors, Ignacio Pagonabarraga and Carlos Calero, for their guidance, support, and continuous and valuable feedback throughout this project.

[1] H. Massana-Cid, D. Levis, R. J. Hernández Hernández, I. Pagonabarraga, and P. Tierno, Physical Review Research **3**, L042021 (2021).
[2] H. Massana-Cid, D. Levis, R. J. Hernández Hernández, I. Pagonabarraga, and P. Tierno, *Supplemental material for: Arrested phase separation in chiral fluids of colloidal spinners* (2021), available as Supplemental Material to Phys. Rev. Research 3, L042021 (2021).

Col·loides rotatoris autoorganitzats en un medi actiu

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Resum: Aquest treball investiga el comportament de partícules col·loïdals passives immerses en un fluid actiu quiralt format per rotors ferromagnètics sotmesos a un camp magnètic rotatori. Mitjançant simulacions numèriques, estudiem com la difusió translacional de les partícules passives es veu influenciada per la freqüència de gir dels rotors, l'alçada vertical respecte una paret amb condició de no lliscament, i l'organització estructural emergent del sistema.

Els nostres resultats mostren que el coeficient de difusió D de les partícules passives depèn fortament tant de la freqüència de gir Λ com de l'alçada h: augmenta linealment a distàncies curtes ($h = 1$), es satura a alçades intermèdies ($h = 2$) i presenta una tendència no monòtona a separacions més grans ($h = 5$). També analitzem la funció de distribució radial per estimar la mida mitjana dels clústers ℓ, i trobem una forta correlació lineal entre ℓ i D, la qual cosa suggereix que l'organització col·lectiva afavoreix el transport. **Paraules clau:** matèria activa, sistemes fora de l'equilibri, clústers, col·loides rotatoris, simulacions

ODSs: Aquest TFG està relacionat amb els Objectius de Desenvolupament Sostenible (SDGs) 4 i 9

Objectius de Desenvolupament Sostenible (ODSs o SDGs)

1. Fi de la es desigualtats		10. Reducció de les desigualtats	
2. Fam zero		11. Ciutats i comunitats sostenibles	
3. Salut i benestar		12. Consum i producció responsables	
4. Educació de qualitat	X	13. Acció climàtica	
5. Igualtat de gènere		14. Vida submarina	
6. Aigua neta i sanejament		15. Vida terrestre	
7. Energia neta i sostenible		16. Pau, justícia i institucions sòlides	
8. Treball digne i creixement econòmic		17. Aliança pels objectius	
9. Indústria, innovació, infraestructures	X		

El contingut d'aquest TFG, part d'un grau universitari de Física, es relaciona principalment amb l'ODS 4, "Educació de qualitat", i en concret amb la fita 4.4, que promou l'adquisició de competències tècniques i científiques en àmbits com la ciència i la tecnologia. El projecte contribueix a la formació acadèmica avançada en física i a l'adquisició de competències en simulació numèrica, anàlisi de dades i recerca científica. A més, està vinculat amb l'ODS 9, "Indústria, innovació i infraestructures", i la seva fita 9.5, que promou la recerca científica i el desenvolupament de capacitats tecnològiques, ja que explora sistemes actius complexos amb potencials aplicacions industrials.

Appendix: Simulation and Analysis Code

The code used to perform the simulations and to compute observables such as the mean square displacement (MSD) and the radial distribution function (RDF) is available at the following GitHub repository:

`https://github.com/PauGrauSabate/TFG`