Projecte de Treball Fi de Màster (TFM)	**Màster en Modelització Computacional Atomística i Multiescala en Física, Química i Bioquímica** UB/UPC

Títol	**Simulació de transport per ratchet en col·loides magnètics**
Title	Simulation of ratchet transport on magnetic colloids

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Universitat	**UB**
Tutor[1]	

Curs	**2023-24**

Summary[2]

The transport of micro and nanoparticles immersed in fluids plays an important role in a range of different fields. Ratchet transport, the rectification of Brownian motion using asymmetric periodic potentials, is a transport strategy effective at these scales which can be used in artificial systems and is also thought to dominate important biological transport processes such as those of molecular motors. In this project we propose to investigate the motion by ratchet transport of a magnetic colloid on top of a chain of paramagnets using numerical simulations. The goal is to characterize with precision the dynamics of the colloidal particle as a function of the actuation and the timescales involved. The results from simulations can be used to understand and propose experiments which are currently being carried over. The conclusions of the study can help to understand open questions regarding ratchet transport relevant for biological systems hard to access experimentally.

Keywords[3] Colloids, ratchet transport, simulation

Breu descripció del projecte[4]

The transport of micro and nanoparticles immersed in fluids plays an important role in a range of different fields, and it is related to a number of potential applications such as drug delivery or microfluidic devices among others. However, achieving net motion at these scales presents specific challenges. At sub-micrometer scales Brownian noise introduces stochasticity into the dynamics of particles and directed motion becomes harder. In addition, the Reynolds number of the induced flow is very small and propulsion cannot be achieved by cyclical reciprocal motions (scallop theorem).

One possibility to achieve propulsion at such scales is the use of Brownian ratchet motors and traveling potentials. Through these mechanisms noise is strategically harnessed to enable motion in a desired direction, often through the utilization of a spatially periodic potential over the transport regime. There exist different realizations of transport through a ratchet mechanism, both artificial and in nature. One example of this concept involves the realization of a flashing ratchet potential using periodically asymmetric geometric patterns etched on surfaces, coupled with electric fields in the transverse direction of motion. This approach proves effective in separating different types of particles in mixtures based on the dependence of diffusion constants on physical properties such as size. In addition, ratchet transport is thought to be the underlying mechanism to explain the dynamics of molecular motors such as kinesin on microtubules. However, there are still a number of open questions regarding the details of such dynamics, which are hard to access experimentally due to the dimensions of the agents involved (at the nanoscale, below visible wavelength).

In this project we plan to investigate the motion by ratchet transport of a magnetic colloid on top of a chain of paramagnets. Under the application of the appropriate external magnetic field the chain of paramagnets creates an asymmetric periodic potential for the magnetic colloid which can rectify Brownian motion if this actuation is alternated with periods of no magnetic field in which the colloid moves stochastically. We plan to characerize with precision the transport of the colloid as a function of both the external actuation (which determines the underlying potential) and the timescales involved. Understanding this colloidal system, which is easier to access in experiment, could help in the understanding of transport of molecular motors.

The methodology of the project is mainly based on numerical simulations of the overdamped Langevin equation. The student will write a code to solve the dynamics of the system and will analyze the different regimes as a function of the parameters of the problem (magnetic field, times of actuation, magnetic susceptibilities of particles). This is a problem with an experimental counterpart which is currently being developed, so the results from the numerical analysis will also be used to propose new experiments.

Tasques a desenvolupar		Cronograma (setmanes)																			
Tasca	Breu descripció	01	02	03	04	05	06	07	08	09	10	11	12	13	14	15	16	17	18	19	20
T01	Bibliographic search (75 h)	X	X	X								X	X				X	X			
T02	Discussion of model of system (25h)		X	X	X																
T03	Implementation of model and simulation code; benchmarking (100h)			X	X	X	X	X													
T04	Performance of simulations (100h)							X	X	X	X	X	X	X	X	X					
T05	Analysis of simulations (50h)										X	X	X	X	X	X	X				
T06	Writing thesis (75h)															X	X	X	X	X	
T07	Preparation of defence (25h)																			X	X
T08																					
T09																					
T10																					

Observacions i comentaris
(EXEMPLE) Per a la realització del treball pròpiament dit es preveu una dedicació d'unes quatre hores diàries durant cinc dies a la setmana, amb la opció de modificació de l'horari per poder adaptar-se millor a l'horari acadèmic de l'estudiant. **COMENTARI: Recordeu que el TFM son 18 ECTS=18*25=450 hores de dedicació de l'estudiant (un 20% han de ser tutelades pel director). Calculeu 18-20 setmanes de març a juny (inclosos) per fer totes les tasques (inclosa la redacció de la memòria).**

Signatura (el director del TFM)

Signatura (el tutor del TFM, si s'escau)

[4] Enumereu breument qualsevol competència addicional a les competències genèriques enumerades en el Pla Docent del TFM (opcional).
[5] Feu servir només les línies que calgui. Escolliu-les de manera que donin una idea aproximada de en què consistirà el treball i la seva distribució temporal.