Projecte de Treball Fi de Màster (TFM)

Màster en Modelització Computacional Atomística i Multiescala en Física, Química i Bioquímica
UB/UPC

Títol	Depleció activa en 2D
Title	Active depletion in 2D

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Universitat	UB
Tutor[1]	

Curs	2023-24

Summary[2]

Equilibrium depletion interactions emerge in systems of colloidal particles of different sizes to maximize the overall entropy of the system. In systems of passive colloids immersed in a bath of active self-propelling particles, forces between the colloids also appear with distinctive and interesting properties. Here we propose an investigation of such emerging interactions as a function of the features of the non-equilibrium active bath. Also, we plan to characterize the aggregation states (the distribution of sizes) which result from such forces. The study is based on numerical simulations of a 2D systems of large passive particles immersed in a solution of smaller self-propelling spherical particles. The analysis will cover systems with different degree of activity and will be based on the characterization of the stationary distributions generated by the presence of the active particles.

Keywords[3] Depletion forces, self-propelling particles, aggregation

Breu descripció del projecte[4]

Depletion forces are effective interactions of entropic origin ubiquitous in colloidal systems when they are immersed in a solution of smaller non-adsorbing particles or polymers (depletants). Depletion interactions in colloids are attractive and arise due to the osmotic pressure difference when depletants are expelled from the region between the colloidal particles. Although in its origin the understanding of depletion interactions is based on thermodynamic equilibrium ideas [1], in recent years there is an important effort to characterize this interaction and its effects in conditions out of equilibrium [2].

In this project we propose to investigate the emerging interactions between large colloids due to their interaction with a bath of smaller particles which can self-propel with velocity v. The study is based on numerical simulations of the active brownian particle (ABP) model, standard to describe the dynamics of particles with propulsion in a thermal bath which induces stochastic forces and torques. Departing from the known case of equilibrium (at velocity of propulsion v=0), we intend to quantify the departure from equilibrium as a function of the activity (the propulsion velocity) of self-propelling depletant particles. To do so we will analyze the effective forces between passive colloids induced by the bath and also the aggregation state of passive colloids. Another possible quantity of interest is the local fluctuation of the density of depletant particles, which exhibits particular properties for active systems and could be important to understand the emergence of active depletion forces.

The methodology of the project is based on computer simulations using both own codes and the simulation package HOOMD, optimized to run in GPUs and with capabilities to use rigid bodies. The student will implement a 2D model of the system containing the active particles (discs) and the larger passive colloids. Using this model, numerical simulations will be performed for a range of activities, departing from the case with no activity (no propulsion velocity, pure diffusive Brownian particle) to a case with high Péclet numbers (which compare the activity and the brownian diffusion effects). Two types of simulations will be performed: (i) simulations with two passive particles at fixed positions to analyze their mutual interaction due to the bath; (ii) simulations with a number of passive particles to characterize the aggregation state due to the emergence of mutual interactions. The case with no activity (which can be approximately solved analytically [3, 4]) can serve as a benchmark of the model and a reference to compare with the cases in presence of activity.

[1] S. Asakura and F. Oosawa, “On interaction between two bodies immersed
in a solution of macromolecules,” The Journal of Chemical Physics 22, 1255–1256 (1954).
[2] Harder, J., et al. "The role of particle shape in active depletion." The Journal of chemical physics 141.19 (2014): 194901.
[3] C. Calero, M. A. Morata, I. Pagonabarraga, “Aggregation of discoidal particles due to depletion interaction” The Journal of Chemical Physics 155.7 (2021): 074904.
[4] C. Calero, I. Pagonabarraga. "Self-Assembly of Microscopic Rods Due to Depletion Interaction." Entropy 22.10 (2020): 1114.

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 active and passive particles (25h)		X	X	X																
T03	Implementation of model and benchmarking (50h)			X	X	X	X	X													
T04	Performance of simulations (100h)							X	X	X	X	X	X	X	X	X					
T05	Analysis of simulations (100h)										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.