Magnetic microrod locomotion in a viscous fluid in rotating field

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Abstract: In recent years the study of propulsion of microparticles immersed in liquids has received a lot of attention. Motivated by experiments carried out by Dr. Pietro's group, we studied the movement of a nickel magnetic filament (specifically a cylindrical microrod) immersed in a viscous fluid with a bounding wall, whose propulsion method will be the application of a rotating magnetic field. The study is divided into two parts: theoretical analysis and motion simulation. The results presented show a strong dependence between the filament/microrod velocity and the frequency and the existence of a critical frequency that we have calculated with theoretical arguments and it agrees with the simulations. Our simulations show a new regime of locomotion which was not proved in experiment.

I. INTRODUCTION

The study of micrometer and nanometer devices in liquids is very important because their applications are many and varied in various fields of science such as the transport of medicines in the human body, microfluidics or their use as non-invasive microsurgical vehicles. Magnetic microswimmers do not require chemical reactions and are relatively easy to control their movement through time-dependent external magnetic fields.

The dynamics of the microswimmers are determined by factors that are not present at the macroscale. The Reynolds number gives us an idea of what dynamics are important (inertial or viscous). Due to the size ($\sim \mu m$) and velocities ($\sim \mu m/s$) involved we are at a very low Reynolds number,

$$Re = \frac{\rho l v}{\eta} << 1 \tag{1}$$

where ρ and η is the fluid density and viscosity respectively, and l and v are the characteristic values of length and velocity of the system. According to Eq. (1) the viscous forces will be much more important than the inertial forces.

The fact that we are at low Reynolds number allows us to neglect the inertial terms of the Navier-Stokes equations (differential equations of fluid velocity). The resulting expression, called Stokes equation, is invariant respect to the time-reversal. This invariance leads to a phenomenology explained by the phenomenon of "scallop theorem" [1]. This theorem tells that if the swimmer performs periodic and symmetric movements, it will not produce net movement. We have to break the spatial symmetry and the temporal reversibility so that the device is propelled in the fluid. One way to achieve this is to place the microdevice near a bounding wall which effectively introduces an asymmetry in the drag with the fluid. Thus, the rotating movement (induced by the magnetic field) together with the presence of the surface will result in a propulsive movement. These are the conditions under which they have done several experiments, among them, those made by Dr. Pietro's group [2].

In this work we study, through numerical simulations and theoretical arguments, the propelling motion of a magnetic microrod in a viscous fluid due to the action of a time-dependent rotating external magnetic field. The rod is located over a bounding surface, which enables the propulsion of the rotating rod due to the hydrodynamic flow that is generated.

The movement of the microrod will take place in the plane of the magnetic field since the rod, being magnetic, will have a magnetic moment trying to align itself with the field, causing a circular rotation in that plane. At the same time we have an opposite hydrodynamic drag due to the fluid. There is a competition between the action of the magnetic torque and the hydrodynamic drag which depends on the frequency of the magnetic field. The presence of a bounding surface affect the friction of the microrod with the fluid which is not the same at each point (there is a dependency on the distance to the surface) allowing its propulsion. Although Brownian motion determines the dynamics of submicrometer swimmers, it is not relevant in the locomotion of micrometer sized particles.

From previous experiments it has been observed that the speed of the swimmer device (microrod) grows linearly with the frequency w of the magnetic field and reaches a maximum speed at a certain value of frequency (critical frequency w_c) over which the speed decreases monotonically to zero, so that for $w \to 0$ and $w \to \infty$, $v = 0$. The general approach of the work would be on one hand to make an analytical estimation of the critical frequency from arguments of stability (equality of torques). On the other hand, we will simulate the microrod dynamics under rotating magnetic fields and also its hydrodynamics. We also explore the range of parameters that constrain the system configuration: length, magnetic field amplitude and rotation frequency.

In section II and III, we will establish the theoretical framework of the dynamics of a magnetic microrod placed near a surface forced by an external magnetic field. In section IV we will present the results using a numeri-

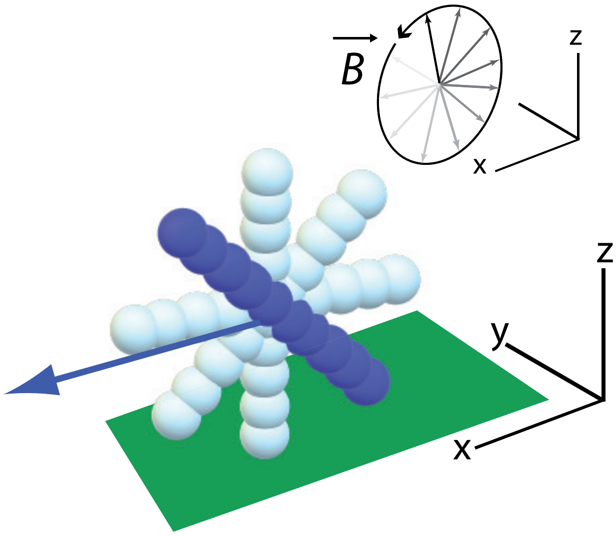

FIG. 1: Three-dimensional representation of the microrod and the components of the magnetic field.

cal approach to solve the dynamics. Finally in section V we will discuss the results and main conclusions.

II. THEORETICAL MODEL

Theoretically what we expect to happen at low frequencies is that the rod will rotate following the magnetic field. As we increase the frequency, the rod rotation velocity will increase. Therefore the hydrodynamic drag will also increase, since it depends on the velocity of the object with respect to the fluid. This behavior will be stable until the hydrodynamic torque of the rod is higher than the torque exerted by the magnetic field on it. At that point, the rod is no longer able to follow the magnetic field and we will have a new regime. These arguments indicate the existence of a critical frequency, for which the hydrodynamic torque is equal to the maximum torque that can be exerted by the magnetic field.

A. Theoretical estimate of the critical frequency

The torque, M_l,exerted by the fluid on a long rod is given by the resistive force theory of an elongated body that can be expressed as [3]:

$$M_l = -\frac{\pi \eta l^3}{3 \log \frac{l}{a}} w_l \tag{2}$$

where w_l is the angular velocity about the z axis, η is the fluid viscosity ($9{\cdot}10^{-4}$ Pa·s in our case) and l and a are the length and the radius of the cylindrical microrod respectively (we use 3 and 0.2 μ-metres respectively). Regarding the magnetic field, the external torque, τ,exerted [4] is:

$$\tau = m_b B_0 \sin \theta, \tag{3}$$

where m_b the magnetization of the microrod (to be assumed constant), B_0 is the magnetic field amplitude and θ is the angle of the rod respect to the magnetic field . In our case we use a circular magnetic field:

$$\vec{B} = B_0(\cos wt, 0, \sin wt) \tag{4}$$

So, using Eq.(2) and Eq.(3) and knowing that critical frequency will correspond to the maximum of the torque exerted ($\theta = 90^o$), we find:

$$w_c = \frac{3}{\pi} \frac{m_b B_0 \log\left(\frac{l}{a}\right)}{l^3 \eta} \tag{5}$$

We see a dependency on the amplitude B_0. This is one of the three parameters that we control in our system (the others are the frequency and the length), so if we increase the magnetic field, we will have a higher critical frequency. The critical frequency also depends strongly on the the length of the rod: the larger the rod the smaller the critical frequency.

III. SIMULATION MODEL

The way we model the system is by decomposing the cylindrical rod in point particles (10 in our case) with spheric form along its axis (Fig.1). Thus we will focus on the movement of each particle and on the forces acting at each point. As we said before, at these length scales, the Reynolds number is very low ($\ll 1$), allowing to eliminate the convective terms of the Navier-Stokes equation; this is the Stokes equation. In our model, we consider the external forces as point forces so the Stokes equations can be solved with the Green's function formalism. The Green's function of the Stokes equation for the velocity field is given by the Blake tensor [5] if no-slip boundary conditions are considered on the plane z=0. This tensor relates the velocity of the fluid at one point with the force exerted on another point. So the velocity field can be expressed as [4] :

$$u_i = \frac{1}{8\pi\eta} \sum_j G_{Blake}(r_i; r_j) \times F_j \tag{6}$$

where u_i is the fluid velocity at each point, $G_{Blake}(r_i; r_j)$ is the Blake tensor (described before) and F_j is the sum of all non-hydrodynamic forces.

A. FORCES

In order to elaborate the dynamics, we first proceed to explain the physical forces involved in the propulsion

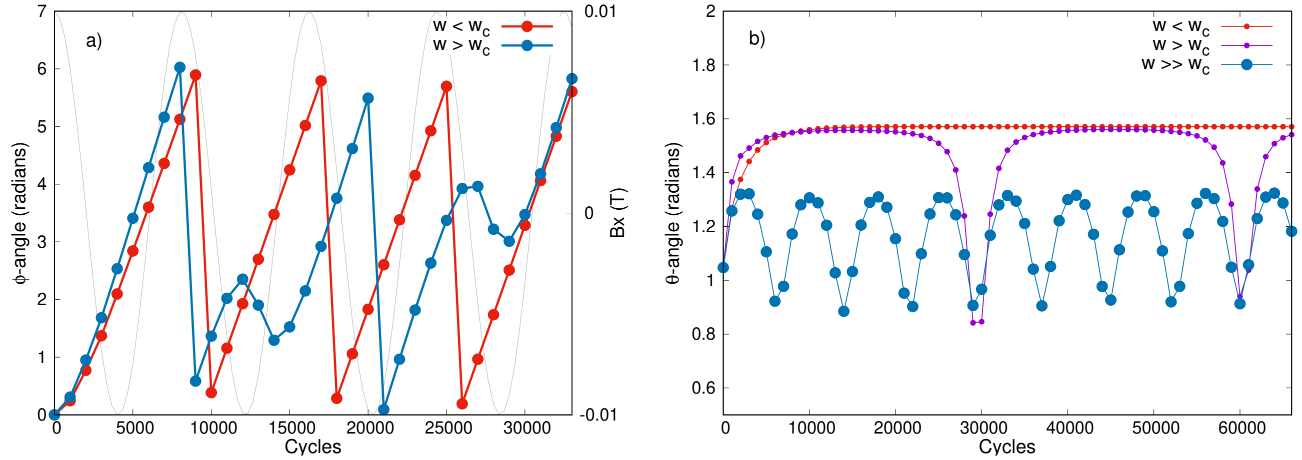

FIG. 2: a) Angle of the microrod respect to the x-axis at frequencies below and above the critical frequency as a function of time (number of cycles). On the other axis, x-component of the magnetic field (grey line) with an amplitude B=10 mT as a function of time (number of cycles). b) Angle of the microrod respect to the y-axis at frequencies below and above and far above the critical frequency as a function of time (number of cycles).

process. On the one hand we have the gravitational force that acts in the Z axis:

$$F_g = -mg\vec{e_z}, \tag{7}$$

where m is the mass of the filament (microrod). We also have the repulsive force of the particles with the plane at Z=0 (Eq. 9), which can be modelled using a Lennard-Jones potential:

$$U_{LJ} = 4\epsilon((\frac{\sigma}{z})^6 - (\frac{\sigma}{z})^{12}) \tag{8}$$

$$F_{LJ} = -\nabla U_{LJ}, \tag{9}$$

where ϵ and σ are constants and z is the distance to the surface. From Eq.(9) we only take the repulsive (positive) part contribution.

Another contribution is the external force due to the magnetic field (Eq.(10)). The magnetic field exerts a torque τ on the ferromagnetic particles, which is modelled as a pair force acting perpendicularly to the axis of the rod, with magnitude:

$$F_B = \frac{1}{2}\frac{\tau}{r_{ji}}, \tag{10}$$

where r_{ji} is the distance between the point i and the point j of the rod. In other words, it is the relative distance between the positions of the particles i and j that form the rod. Finally, we have the friction force because the nanoswimmer is immersed in a viscous fluid:

$$F_f = -\gamma(v_i - u_i), \tag{11}$$

where v_i is the speed of the rod at that point and u_i is the fluid velocity at that point which is given by Eq. (6).

B. MODEL EQUATIONS

In order to write the motion equations for the microrod, we will separate the hydrodynamic forces (friction) from the non-hydrodynamic ones (gravitation, potential repulsion and magnetic field) $\overline{F}_i$, i.e, the forces that depend on the speed and those that do not.

$$m\frac{dv_i}{dt} = \overline{F}_i - \gamma(v_i - u_i), \tag{12}$$

The dynamics of the particles, Eq. (12), is solved with an adapted version of Verlet's algorithm for velocity-dependent forces [6]:

$$r_i(t+dt) = r_i(t) + v_i(dt)\cdot dt + \frac{dt^2}{2m}F_i(t), \tag{13}$$

$$v_i(t+dt) = \frac{2m-\gamma dt}{2m+\gamma dt}v_i(t) + \frac{dt}{2m+\gamma dt}[\overline{F}_i(t) + \overline{F}_i(t+dt)], \tag{14}$$

IV. RESULTS

A. Initial configuration XZ

The first case that we have considered is an initial configuration where the microrod was initially in the XZ plane, forming an angle of 30º with the x-axis (without y-component). This case is pathological because the rod motion at any frequency is restricted to the XZ plane and does not allow any movement out of it.

The velocity has two different behaviours separated by the critical frequency w_c. For $w < w_c$, the velocity is linear with the frequency of the magnetic field. In contrast for $w > w_c$ the velocity decreases monotonically to

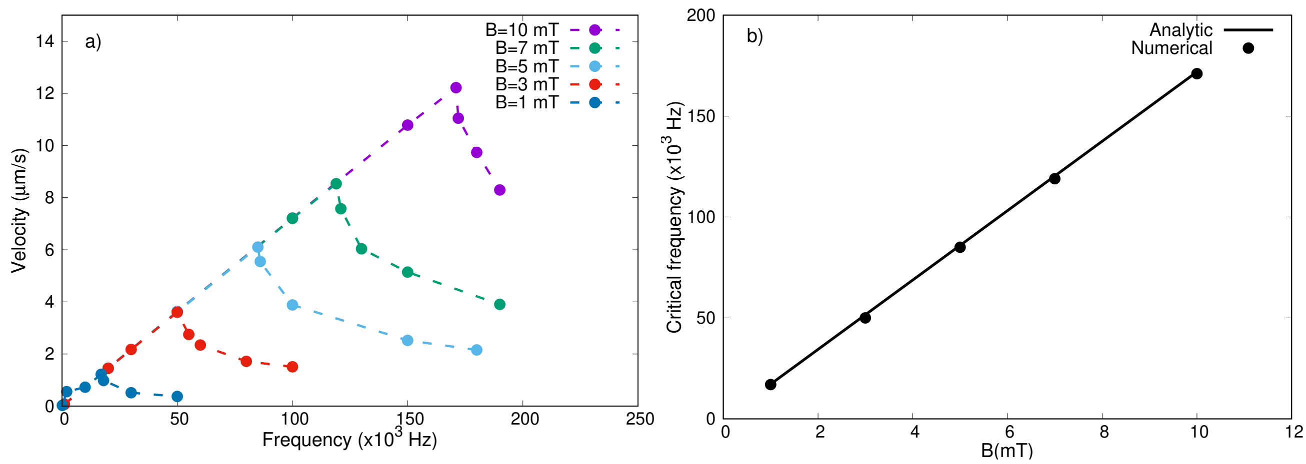

FIG. 3: a) Microrod velocity along x-axis as a function of the frequency for different values of the magnetic field amplitude. b) Critical frequency dependence on the magnetic field amplitude.

zero. This behaviour can be explained by the fact that from the critical frequency w_c onwards the microrod is no longer able to follow the magnetic field well because it is going too fast. At this moment the hydrodynamic torque (friction) is more important than the magnetic torque causing a loss of velocity in the microrod. The circular movement of the filament observed in the simulation is affected by a small circular repetition movement in the opposite direction, which is more pronounced as we move further and further away from w_c. This behaviour can be seen in Fig. 2 a), where we see how the angle of the rod changes with respect to the x-axis. At $w < w_c$, the rod rotates normally; it starts at angle 0 (horizontal rod), increases until it reaches 2π radians (take a full turn) and starts all over again. On the other hand, for $w > w_c$ the rod also starts with angle $\phi = 0$ but at a given moment the angle decreases instead of increasing. This corresponds to the situation where the rod cannot follow the magnetic field and it is more favourable for it to rotate backwards than forwards.

B. Initial configuration on the XY plane

The second case considered is one where, initially, the ferromagnetic rod is located on top of the bounding XY plane forming an angle (of 30° in the examples shown below) with the x-axis. This configuration is very similar to the situation studied in previous experiments (three-dimensional plane)[2] .

The results are practically the same as the previous case, i.e we also have two different behaviours (Fig.3 a)) for high and low frequencies. The numerical value of the critical frequency (depending on the magnetic field amplitude) calculated from the simulation and the values calculated analytically (Fig.3 b)) are practically the same which tells us that the numerical model fits very well to the theoretical model made in this work. For $w < w_c$ the speed behavior is linear with respect to the frequency and the rod rotates in the XZ plane. The microrod rotates circularly in the XZ plane with a net movement along the x-axis. Also, as shown in Fig. 3 a), in this regime the rod rotates with the magnetic field and faster rotations induce higher velocities. However, for $w > w_c$ the velocity decreases and an important change in the motion is observed with respect to the previous case, since the rod presents a conical movement composed of oscillating motions in the XY and the XZ planes. This is shown in Fig. 2 b), where at low frequencies the angle of the rod with the y-axis is always the same ($\frac{\cdot\pi}{2}$ radians) because its motion does not leave the XZ plane, but at high frequencies (over the critical) it is out of this plane (movement in XYZ plane). The conical movement develops because it lowers the hydrodynamic drag as the angle θ decreases. Furthermore, this conical motion is progressive so that, near the critical frequency, it appears sometimes, but it becomes more and more periodic at higher frequencies. This implies that there is a "transitional regime" for frequencies that are higher than critical but not yet very far away. It is important to remark that this "transitional regime" (regarding the frequency) has not been observed in the previous experiments. The reason is because the movement of the rod at all frequencies could not be observed.

C. Larger dimensions

The results of the velocity calculations shown above correspond to rods significantly smaller than those used in the experiments done by J. Vila [2]. Therefore, larger rod lengths have been explored to obtain more results closer to the experimental range. This is shown in (Fig. 4) where you can see that the effect of making the rod larger makes the frequency range (where the movement takes place) smaller (from Eq. (5) we see that $w_c \propto \frac{1}{l^3}$).

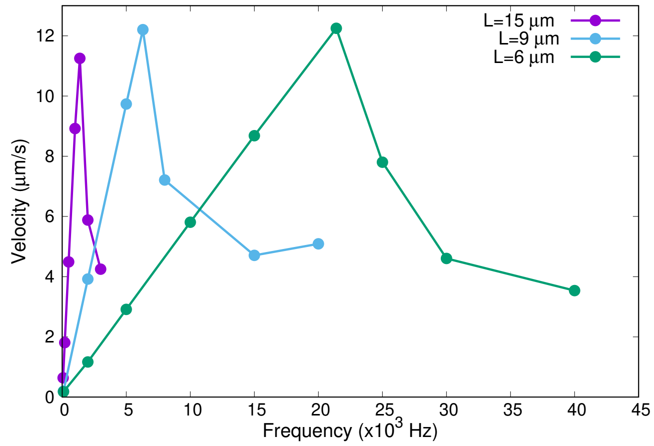

FIG. 4: Velocity along x-axis depending on the frequency at B=10 mT, for different lengths of the microrod.

Even so, you can see that the maximum velocity reached is more or less the same for every length since we are applying the same field for all of them. Simultaneously, both the velocity profile and the rod movement are also the same for every length. In addition, for L=15 μm we have seen a change in the movement direction for very low frequencies (not observed for shorter lengths) due to the action of gravity.

V. CONCLUSIONS

In this work, we have simulated the movement of a magnetic microrod immersed in a viscous fluid with the presence of a bounding surface in XY plane (Z=0). The initial configurations have been, one where the rod is forming a 30 degree angle in the XZ plane (without an Y component) and a second one where the rod is forming the same angle but in the XY plane. The first one is a simple unrealistic case while the second one is close to the experiments since it allowed a three-dimensional movement for high frequencies.

The results regarding the velocities are qualitatively in agreement with the experiments carried out by Dr. Pietro's group [2] , showing a linear dependence with frequency for $w < w_c$ and a monotonous decay for $w > w_c$. Furthermore the theoretical estimation of the critical frequency fits very well with the numerical results. Even so, it has not been possible to replicate exactly the experimental values since we have used dimensions of the rod different as those used in the experiments. Regarding the motion, the simulation reproduces exactly the same movement regimes seen in the experiments. For $w < w_c$, the microrod rotates in the same direction as the magnetic field and is propelled along the x-axis (XZ plane). For $w > w_c$ the rod has a three-dimensional conical motion composed of oscillating motions in the XY and the XZ planes. Furthermore, it has been seen that this three-dimensional movement is not periodic till frequencies far from the critical ($w >> w_c$). Therefore it appears a "transitional regime" not observed in the experiments (they have not been able to observe in detail the movement of the rod for all frequencies).

Regarding the dimensions of the rod, we have seen that the behaviour of the velocity with respect to the frequency and the rod motion for larger dimensions is the same. It has also been observed that for the maximum length simulated in this work (15 μm) at very low frequencies, the rod changed its direction of movement due to the action of gravity.

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