Hydrodynamical random walker with chemotactic memory

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A three-dimensional hydrodynamical model for a micro random walker is combined with the idea of chemotactic signaling network of E. coli. Diffusion exponents, orientational correlation functions and their dependence on the geometrical and dynamical parameters of the system are analyzed numerically. Because of the chemotactic memory, the walker shows superdiffusing displacements in all directions with the largest diffusion exponent for a direction along the food gradient. Mean square displacements and orientational correlation functions show that the chemotactic memory washes out all the signatures due to the geometrical asymmetry of the walker and statistical properties are asymmetric only with respect to the direction of food gradient. For different values of the memory time, the Chemotactic index (CI) is also calculated.

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I. INTRODUCTION

Random walk as a general mathematical tool can describe a large class of biophysical systems such as the motion of Brownian colloidal particles and the motion of biological self-propelled microorganisms [1–6]. Passive colloidal particles in response to the thermal forces randomly change their directions but microorganisms sense the directions and overcome the thermal randomness to reach a predefined target point. Microorganisms do not have a complex intelligence in the form of a brain that can process the complicated signals from different senses. Chemotaxis is a mechanism that microscopic organisms use to detect their right tracks and navigate toward their targets [7–10]. The phenomenon of chemotaxis has inspired extensive research both due to its direct biological relevance [11–13] and also because of the practical needs for designing artificial nanorobots that can sense the direction [14, 15]. As the swimming of bacteria takes place in aqueous media, the inertialess condition in microscopic world results a peculiar fluid dynamic problem [16]. From the other hand, at the scale of micrometer, the fluctuations are the non negligible part of the physics and any kind of modeling should take into account the effects due to randomness. Mathematical description of chemotaxis in terms of random walk requires a knowledge about the values of jumping displacements and rotations and their transition probabilities.

So far, theoretical studies on random walk modeling for microorganisms do not consider the hydrodynamical details and also the mechanism of chemotactic memory in a unified model. In this article, we aim to construct a model that takes into account the details of hydrodynamical displacements, mechanism of chemotaxis memory and also the physics of fluctuations. This model will exhibit detailed features of the motion that provides a coupling between the geometrical parameters of the walker with the conformational rates. Geometrical parameters contribute through the hydrodynamic part and the dynamical parameters will enter through the chemotactic memory mechanism.

The structure of this article is as follows: In section II we introduce the hydrodynamical details of the system and the chemical mechanism for the memory of the swimmer will be studied in section III. Finally the statistical results based on numerical investigations will be presented in section IV.

II. HYDRODYNAMICAL MODEL

Our goal in this article is to combine the idea of chemical memory with a hydrodynamical model of a walker. Now let us introduce the hydrodynamical details of our system. Inspired by a Bacterium, Fig. 1(a) shows the body of our walker that is modeled by a sphere of radius \( R \). The driving force is modeled by a mobile small sphere with radius \( a \) \((a \ll R)\). These two spheres are connected by an arm with negligible diameter. This model resembles the geometry of a bacterium with a single tail. As shown in this figure, and in a reference frame connected to the large sphere, jumps of this small sphere between 4 vertices of a pyramid will construct all internal discontinues jumps of the walker. The apex of this pyramid is a point with a distance \( L \) apart from the large sphere and is chosen as state (1). The other 3 states are located on the base of this pyramid. The apex angle is \( 2\phi \) and the apex sides are \( \varepsilon \). The base of this pyramid is an equilateral triangle with sides \( 2\varepsilon \sin \phi \). The angle \( \phi \) may resemble the amplitude of flagellum undulations. The hydrodynamic question that we need to address here, is the differential change of the position and orientation of the system for an internal jump. For a fluid with viscosity \( \eta \) and at the condition of micron scale, the inertialess stokes equation \( \eta \nabla^2 \mathbf{u} - \nabla P = 0 \), written for the fluid velocity \( \mathbf{u} \) and pressure \( P \), describes the dynamics. The condition of incomprehensibility, should also be considered. A prescribed motion corresponding to a jump of
the small sphere, will enter to the dynamics through the boundary conditions. Solving the Stokes equation with the corresponding boundary conditions would result the dynamical properties of the large sphere during an internal jump. Calculations similar to the details presented elsewhere, reveals the dynamical results [22]. To summarize the hydrodynamical results, let’s denote the relative scale can be defined as: \( \tau^H = \varepsilon / v \). This is the time for jumps that start from the apex and a jump in the base face of the pyramid. Other jumps can be obtained from these two special jumps by applying the appropriate rotation matrices. Symmetry requires that \( \tilde{\omega}_{ij} = -\tilde{\omega}_{ji} \) and \( \delta \tilde{x}_{ij} = -\delta \tilde{x}_{ji} \). A hydrodynamic time scale can be defined as: \( \tau^H = \varepsilon / v \). This is the time for jumps that start from the apex of pyramid, the time for other jumps are given by: \( 2 \tau^H \sin \varphi \).

In the next section we first introduce the chemotactic memory of a bacterium then show how can we combine the idea of chemotactic memory with the above introduced hydrodynamical swimmer.

### III. CHEMOTACTIC MEMORY

To have a plan for internal jumps, we use the chemotactic strategy that bacteria use to navigate. Among different microorganisms, the chemical network responsible for chemotactic signaling is well understood and studied in E. coli [17, 18]. Running state of this bacterium is due to the CCW (counter clockwise) rotation of flagella and changing the flagellar rotational state to CW (clockwise) will result a tumble. Chemical signals inside cell, controls the frequency of these running and tumbling states. A very simplified picture of different proteins involved in the chemical signal transduction pathway is shown in Fig. 1(c). Two important processes of phosphorylation and methylation take place inside cell. Phosphorylated CheY-P enzymes produced by cheA (enzymes connected to receptors), are responsible to enhance the rotational direction of flagella and subsequently force bacterium to tumble. Methylation level of receptors from one hand and the concentration of the food from other hand, change the activity of receptors and enhance the phosphorylation process. (d) Subsequent runs and tumbles would lead the bacterium to find the source of food.

\[
\begin{align*}
\delta \tilde{x}_{12} &= \left( -\delta \sin \varphi \quad \delta' \quad \frac{\delta}{\sqrt{3}} \sin \varphi \right), \\
\delta \tilde{x}_{24} &= \left( \frac{\delta}{2} \quad 0 \quad \frac{\delta}{\sqrt{2}} \right),
\end{align*}
\]

where the parameters are defined as:

\[
\alpha = \frac{3}{8} \left( \frac{\varepsilon}{R} \right) \left( \frac{a}{R} \right) (1 + \frac{L}{R}), \quad \delta = \left( \frac{\varepsilon}{R} \right) \left( \frac{a}{R} \right) (1 - \frac{3}{4} \frac{R}{L}),
\]

\[
\delta' = \left( \frac{\varepsilon}{R} \right) \left( \frac{a}{R} \right) (1 - \frac{3}{4} \frac{R}{2L}) \sqrt{1 - \frac{4}{3} \sin^2 \varphi}.
\]

Please note that the results are presented for a walker with \( \varepsilon \ll L \). The differential changes are given only for two jumps, a jump started from the apex and a jump in the base face of the pyramid. Other jumps can be obtained from these two special jumps by applying the appropriate rotation matrices. Symmetry requires that \( \tilde{\omega}_{ij} = -\tilde{\omega}_{ji} \) and \( \delta \tilde{x}_{ij} = -\delta \tilde{x}_{ji} \). A hydrodynamic time scale can be defined as: \( \tau^H = \varepsilon / v \). This is the time for jumps that start from the apex of pyramid, the time for other jumps are given by: \( 2 \tau^H \sin \varphi \).

In the next section we first introduce the chemotactic memory of a bacterium then show how can we combine the idea of chemotactic memory with the above introduced hydrodynamical swimmer.
random walker that has no chance to sense the direction of gradient. What we want to consider, is a sort of an intelligent walker that can dynamically change its jumping probabilities. In comparison with E. coli, we first define a set of jumps that corresponds to a CW rotation. We define all the following jumps as CW jumps: 1 \rightarrow 2, 2 \rightarrow 3, 3 \rightarrow 4, 4 \rightarrow 2.

In Fig. 2(b), all these CW jumps, are shown. After defining CW jumps, we assume that the probability for any CW jump is given by a response $S(\vec{r}, t)$ from a chemotactic memory, and other jumps are determined randomly so that:

$$P_{ij} = \begin{cases} S(\vec{r}, t), & \text{if } S(\vec{r}, t) \geq \frac{\xi}{H}, \\ \frac{1-S(\vec{r}, t)}{2}, & \text{otherwise.} \end{cases}$$

Here $\vec{r}$ is the position of the walker at time $t$. Similar to the chemotaxis signaling network of E. coli, we assume that the signal $S$, is connected to the source $c$ (the local concentrations of food) through an intermediate dimensionless memory function $m$:

$$S(\vec{r}, t) = \xi \left( 1 + \exp\left[ v_0 c(\vec{r}) \right]\right).$$

The dynamics of memory function is given by:

$$\dot{m}(\vec{r}, t) = (\tau^H / \tau_{ch})(S(\vec{r}, t) - \xi/3),$$

where the dimensionless time scale of the adaptation is given by $\tau_{ch}/\tau^H$ and $v_0$ is a constant that has the dimension of volume. For a uniform profile of the concentration, this system reaches a steady state with $S^*(\vec{r}, t) = \xi/3$. Here $\xi$ is a parameter in the interval $[0, 1]$ and it shows how the internal jumps of the walker is anisotropic in the absence of any food gradient. Throughout this paper we will choose $\xi = 0.95$. For a nonuniform concentration profile, there is no static steady state solution and the system evolves in time by continuously adjusting its relative position and orientation with respect to the concentration profile.

The statistical properties of this swimmer will be studied in details in the next section.

IV. RESULTS

Fig. 2(a) shows a typical trajectory of the walker in a uniform concentration profile of food molecules. It represents the trajectory of a random walker. To study the effect of a nonuniform concentration we choose a linear gradient in $x$ direction. Throughout this paper, and for nonuniform concentration, we choose a linear gradient with $v_0 c(\vec{r}) = 100x/R$. A typical trajectory for the walker moving in this concentration field is shown in Fig. 2(b). As one can see, the subsequent tumbles bias the trajectory toward the place with larger concentration of food molecules. In the literature of chemotaxis, $CI$ the chemotactic index is an important quantity that shows how accurate is a direction sensing mechanism. It is defined as the ratio of the walking displacement along the concentration gradient to the total length of the walking trajectory. Depending on the dynamical variables of the system, $CI$ belongs to the interval $[-1, 1]$. In Fig. 3, $CI$ is plotted in terms of the dimensionless memory time $\tau_{ch}/\tau^H$. Here $\tau_{ch}$ is a parameter that comes from the chemical dynamics and $\tau^H$ is a geometrical parameter. For large memory times ($\tau_{ch} \geq \tau^H$), the chemotactic index is positive. This is a signature saying that the chemotactic mechanism has a positive overcome and the walker can successfully reach the target, the place of more food. As the time scale for a single jump is given by $\tau^H$, this proves that $\tau_{ch}$ plays the role of a memory time. The memory time should be greater than the individual jumping time and this is the only condition required to have a successful gradient sensing walker. The $CI$ is calculated for two different values of the apex angle. It is seen that the overcome of the searching mechanism is not so sensitive to this angle. Now we can study the statistical properties of the system for $\tau_{ch} \geq \tau^H$. To have a better understanding of the role of fluctuations, we repeat the simulations for an ensemble of walkers and have studied.
FIG. 4: Statistical properties of walkers moving in either a uniform concentration or a concentration with a linear gradient. Part (a) shows average position of the walker as a function of time. As one can see a concentration with gradient in the $x$ direction will result an average swimming to the positions with higher concentration of food. (b) shows the short time behavior of mean square displacement in terms of time and (c) shows the corresponding behavior at large time scales. The chemotaxis memory shows positive results only at large time scales. For a walker moving in uniform concentration, the long time and short time behaviors are separated by a nonlinear crossover. This reflects the non symmetric nature of our passive walker. The numerical parameters are as in Fig. 2.

the average statistical properties of the system. Mean displacement (MS), mean square displacements (MSD) and correlation functions are the statistical variables that we consider. To quantify the results of MSD, we define the diffusion exponents as:

\[ \langle x^2 \rangle \sim t^{\nu_{\parallel}}, \quad \langle y^2 \rangle = \langle z^2 \rangle \sim t^{\nu_{\perp}}, \]

where $\nu_{\parallel}$ and $\nu_{\perp}$ are the diffusion exponents along the gradient and along a direction perpendicular to the gradient, respectively. For a symmetric and normal random walker we have: $\nu_{\parallel} = \nu_{\perp} = 1$. MD for a random walker moving in uniform and nonuniform concentration profiles are presented in Fig. (a). As we expect, for nonuniform concentration the characteristics of a random walker is recovered, but for a nonuniform concentration with a gradient in $x$ direction, the walker is biased toward the positive $x$ direction. For nonuniform concentration, MD in the perpendicular directions ($\langle y^2 \rangle$, $\langle z^2 \rangle$) are zero but it is not zero in the direction of gradient ($\langle x^2 \rangle$).

MSD in terms of time, in logarithmic scale, shows a nonlinear crossover from a short time to long time behavior. Figures (b) and (c) show the short and long time MSD results for this walker. This crossover is a result of the hydrodynamical anisotropy of the system. Please note that our system, spherical body with a connected tail, is anisotropic. A similar crossover is recently observed for a diffusing object with boomerang geometry \[24\].

FIG. 5: Orientational correlation function is plotted as a function of time. Here $\theta_x(t)$, is the angle that the director vector of walker makes with the $x$ axis of the laboratory frame. Correlation time is sensitive on the geometrical variable (here $\varphi$) of the walker. For larger apex angle, the correlation function for a nonuniform gradient is larger than the corresponding value in uniform concentration. The dashed line shows the complete uncorrelated state with correlation $\pi^2/4$. The numerical parameters are as in Fig. 2.

where $\theta_x(t)$ represents the angle that the director of the walker makes with $x$ axis (parallel to the concentration gradients). Fig. (c) shows the features of the correlation function for walkers moving in uniform and nonuniform concentrations. Correlation time, the decay time for the correlation, is sensitive to the apex angle. For larger apex angles, the correlation time is also larger. This graph shows that the crossover time is essentially the time that orientational correlation washes out.

In conclusion, we have considered the statistical properties of a model hydrodynamical walker moving in a gradient field of food. Nontrivial coupling of geometrical pa-
parameters with dynamical parameters, reveals interesting statistical properties of the walker. The memory time that is introduced within chemotactic mechanism, makes a superdiffusion walker. A crossover from a short time to long time behavior of MSD is observed and the crossover time is the orientational correlation time. The hydrodynamic interaction between different walkers, is shown to have interesting features [26]. Along the extension of this work, we are considering the role of hydrodynamic couplings in the physics of chemotaxis.

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