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学位の種類	博士(理学)
学位記番号	理学博 第9号
学位授与の日付	令和3年3月25日
課程・論文の別	学位規則第4条第1項該当
学位論文題名	Theoretical study on self-propulsion and state transition of micromachines マイクロマシンの自己推進と状態遷移に関する理論的研究(英文)
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【論文の内容の要旨】

Micromachines are tiny machines, such as motor proteins, metabolic enzymes or motile bacteria. All of the micromachines show net functions in overdamped situations, and are expected to be relevant to microfluidics and microsystems. By transforming chemical energy into mechanical work, micromachines show various non-equilibrium behaviors. Recently, these behaviors have attracted great interests both experimentally and theoretically.

First, I discuss the locomotion of a three-sphere microswimmer in a viscoelastic medium and propose a new type of active microrheology. I derive a relation that connects the average swimming velocity and the frequency-dependent viscosity of the surrounding medium. In this relation, the viscous contribution can exist only when the time-reversal symmetry is broken, whereas the elastic contribution is present only when the structural symmetry of the swimmer is broken. Purcell's scallop theorem breaks down for a three-sphere swimmer in a viscoelastic medium.

Next, I propose a model of three-disk micromachine swimming in a quasi two-dimensional supported membrane. I calculate the average swimming velocity as a function of the disk size and the arm length. Due to the presence of the hydrodynamic screening length in the quasi two-dimensional fluid, the geometric factor appearing in the average velocity exhibits three different asymptotic behaviors depending on the

microswimmer size and the hydrodynamic screening length. This is in sharp contrast with a microswimmer in a three-dimensional bulk fluid that shows only a single scaling behavior. The intrinsic drag of the disks on the substrate does not alter the scaling behaviors of the geometric factor.

Then I discuss the locomotion of a three-sphere microswimmer in a viscoelastic structured fluid characterized by typical length and time scales. I derive a general expression to link the average swimming velocity to the sphere mobilities. In this relationship, a viscous contribution exists when the time-reversal symmetry is broken, whereas an elastic contribution is present when the structural symmetry of the microswimmer is broken. As an example of a structured fluid, I consider a polymer gel, which is described by a “two-fluid model”. I demonstrate in detail that the competition between the swimmer size and the polymer mesh size gives rise to the rich dynamics of a three-sphere microswimmer.

After that, I discuss the dynamics of a generalized three-sphere microswimmer in which the spheres are connected by two elastic springs. The natural length of each spring is assumed to undergo a prescribed cyclic change. I analytically obtain the average swimming velocity as a function of the frequency of cyclic change in the natural length. In the low-frequency region, the swimming velocity increases with frequency, and its expression reduces to that of the original three-sphere model. Conversely, in the high-frequency region, the average velocity decreases with increasing frequency. Such behavior originates from the intrinsic spring relaxation dynamics of an elastic swimmer moving in a viscous fluid.

In the latter part of the thesis, I propose a model that describes cyclic state transitions of a micromachine driven by a chemical reaction. I consider the dynamics of variables representing the degree of chemical reaction and the state of a micromachine. The total free energy of the system is the sum of the tilted periodic potential and the periodic coupling energy. I assume that the reaction variable obeys a deterministic stepwise dynamics characterized by two characteristic times: the mean first passage time and the mean first transition path time. To quantify the functionality of a micromachine, I introduce a physical quantity called “state cyclone” and further discuss its dependency on the properties of the chemical reaction. For example, I show that the state cyclone is proportional to the square of the mean first transition path time. The explicit calculation of these time scales reveals that the state cyclone is inversely proportional to the square of the activation energy of the chemical reaction.

Finally, with the use of the “two-fluid model”, I discuss anomalous diffusion induced by active micromachines in viscoelastic media. Micromachines, such as proteins and

bacteria, generate non-thermal fluctuating flows that lead to a substantial increment of the diffusion. Using the partial Green's function of the two-fluid model, I calculate active (non-thermal) one-point and two-point correlation functions due to active force dipoles. The time correlation of a force dipole is assumed to decay exponentially with a characteristic time scale. I show that the active component of the displacement cross-correlation function exhibits various crossovers from super-diffusive to sub-diffusive behaviors depending on the characteristic time scales and the particle separation.