

Doctoral Thesis

**Dynamics of
active deformable particle**

**—Two types of active spinning motions
and dynamics in external flow field—**

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Abstract

This thesis concerns the dynamics of active deformable particles. Active matter is an object that exhibits spontaneous movements, and therefore varies from biological living organisms to synthetic materials. Major part of synthetic active matters is rigid, but there also exist soft active matters that do change the shape during their movements. Such deformability is of basic importance for many biological living creatures.

We develop theoretical investigations into the dynamics of active deformable particles by using model equations derived from symmetry arguments. In order to describe deformation of the particle, we employ symmetric deformation tensors. The expression of the deformation tensors enables us to take deformation into account systematically. In a similar way, the rotation of the particle is described by an antisymmetric tensor of second order. We consider a particle in an external flow field and introduce time-evolution equations for the centre-of-mass position and velocity vector variables, the symmetric tensor variables representing the shape deformation, and the antisymmetric tensor variable characterising the rotation of the particle. In particular the following two situations in a two-dimensional space are studied in detail.

First, we consider the dynamics of active deformable particles in a quiescent flow field, where we concern a spinning motion. We propound the argument that, when the particle is deformable, there are at least two types of spinning motion. One is a spinning motion due to the rotation of the whole body. Therefore this corresponds to the spinning motion of a rigid particle. The other is related to the deformation of the particle shape. When the particle is deformable, the deformation is not necessarily static but can change in time. Then the shape deformation may travel along the interface of the particle. In terms of the dynamics of the particle, this traveling wave of deformation is regarded as a spinning motion. Since this spinning motion does not require the rotation of the whole body, we argue it is a different dynamical mode from the other spinning motion. We verify this proposition by introducing model equations for each spinning motion and developing analytical and numerical investigations.

Second, we study the dynamics of active deformable particles in an external flow field. Particularly two flow geometries are considered as examples. On the one hand, a linear shear flow is taken into account as one of the simplest flow geometries. For a small shear rate, the active particle undergoes dynamical motions that the particle exhibits spontaneously in the absence of the external flow, in addition to the transport by the external flow field, resulting, for instance, in a cycloidal trajectory. Increasing the shear rate, the dynamics of active deformable particles become more complicated, so

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that regular and undulated cycloids, winding motions and even chaotic behaviours are obtained. Interestingly, when the particle either does not exhibit rotation spontaneously or does rotate spontaneously in the opposite direction to the rotation due to the external shear flow, it undergoes an active straight motion for large shear rate, unlike the particle that spontaneously rotates in the same direction as the rotation due to the external shear flow.

On the other hand, a swirl flow is taken into consideration. Astonishingly the motion of active particles in a swirl had never been considered before our study, although swirl flows occur quite naturally in many situations, including turbulence. Since the flow profile of a swirl is similar to that of a scattering geometry and possesses therefore analogy to the classical Kepler and Rutherford problems, we investigate an analogous setup in the context of active particles. We prepare self-propelled particles heading towards the vortex center, and observe the subsequent capturing and scattering dynamics. We distinguish between two major types of active deformable particles, those that tend to elongate perpendicularly to the propulsion direction and those that pursue a parallel elongation. While the former ones either were scattered or get caught by the swirl, the latter ones were always scattered, which proposes a promising escape strategy.

Since the equations of motion we consider in this thesis are derived from symmetry considerations and hence, no detailed mechanism are required to be specified, the obtained results should be general. It is of great importance to understand basic dynamical motions and clarify their origin by using simple models because it is expected to provide a key route to elucidate more complicated dynamics in real systems.

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Chapter 1

Introduction

Physics of active matter has attracted much attention from the viewpoint of various orders of far from equilibrium. A brief definition of active matter is an object that moves spontaneously by generating kinetic energy in itself. Examples thus include both biological and artificial systems. Therefore, besides detailed modelling of each specific system, theoretical modelling from a broad viewpoint is necessary to clarify universality of active matter.

The emergence of new dynamical motion is accompanied by symmetry breaking. Active matter usually contains several types of internal degrees of freedom, which play important roles for the spontaneous movements. Due to the internal structure of the active matter, its dynamics becomes more complicated. To reveal new dynamical states of active matter, theoretical analysis of nonlinear dynamics and non-equilibrium statistical physics are required to be developed. The aim of this thesis is to clarify the role of shape deformation in the dynamics of active deformable particles systematically.

1.1 Active particle

Active matter is an object composed of self-driven units, or *active particles*,¹ which possess internal mechanisms to convert potential energy such as chemical energy into systematic movement [1, 2]. In addition, active particles are accompanied by mechanisms for energy dissipation to stabilise their spontaneous movements. Therefore, active particles and hence active matters are already by definition systems far from equilibrium. This makes it attractive and important in the field of far-from-equilibrium physics.

Due to the kinetic energy generated in it, active matter exhibits various types of dynamical motions. The motion that active matter spontaneously exhibits is referred to as active motion. Among active motions, there are several types of dynamical movements: a spontaneous translational motion, a spontaneous rotational motion (spinning motion), a spontaneous deformation, and fission and fusion of active particles.²

¹Therefore, a single active particle is already one active matter. The size scale of the self-driven unit or the active particle may vary depending on the system of interest.

²These active motions are what we consider in this thesis, except the fission and fusion of active matter.

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As we will see below, examples of active matter are observed from biological living systems to artificial materials. Furthermore, the internal mechanisms relevant to active motions vary from chemical reactions on the interface to more complicated processes inside the particle. Despite its diverse realisation, the concept of active matter provides an opportunity to consider biological and artificial systems on the same stage. In other words, active matter enables physicists to find a route to approach biological problems. One possible goal of active matter physics is to bridge material science, which has been studied in the field of soft condensed matter physics, and biological organisms. A number of researchers of soft matter physics have started to enter the field of active matter, dealing mainly with the mechanics of artificial active matters [3] but also with soft matter physics in biological settings such as a bacterial bath [4, 5].

Besides, other researches on active matter are trying to understand physical aspects of living matters [2, 6, 7]. In the case of living active matters, the internal mechanisms that give the emergence of active processes are usually more complex than artificial active matters, and on top of it they are strongly coupled to macroscopic dynamics of the living organisms [8]. Therefore, dynamics of the internal structures of living matter such as polymerisation process of actin filaments has already been one research field [6, 9]. Numerical simulations to combine the internal polymerisation process to the cell movement have recently been developing [10–12]. However, a systematic theoretical description of active matters including the internal energy-transducing mechanisms is not yet developed for both artificial and biological systems.

1.2 Example of active particle

Active matter includes miscellaneous biological systems and great effort has been paid to develop various types of artificial active matters as well [13]. Here we would describe some of the realisations of active matter.

Examples of active matter are found in a variety of biological processes and living systems. Smallest elements of biological active matter may be molecular motors, or motor proteins [14–16], and biofilaments, which undergo polymerisation and depolymerisation process known as treadmilling [17]. For both of them, adenosine triphosphate (ATP) plays an important role. Cytoskeleton is basically the mixture of these two elements, which is also studied as active gel [18, 19]. Such mechanism is contained in living cells, which actually enables the cells to exhibit dynamical motions spontaneously [20–22]. A cell itself is thus regarded as an active matter, or an active particle. Indeed, living cell dynamics is one of the attractive and difficult research subjects in the field of active matter physics. Of course the polymerization is not the only internal mechanism of living organisms, and they further have for instance sensing mechanisms, which affect their macroscopic movements. The existence of various internal degrees of freedom makes the dynamics of active matter interesting and complicated.

Artificial active matters are also realised experimentally. Major and well-studied part of artificial active matter is colloidal systems [23]. Janus colloidal particles, on the surface of which one side has different properties such as a chemical property from the

other, spontaneously creates e.g. a gradient of chemical concentrations [24] or a thermal gradient [25]. Due to the induced anisotropy, active colloidal particles experience a translational motion spontaneously [26, 27]. See Ref. [3] for more descriptions about active colloids.

Much simpler artificial active matter is a camphor boat.³ Camphor solid floating on a water surface is well studied experimentally [28–32], where they clarified that the shape of the particle affects its dynamical motion. For example, the particle spontaneously undergoes a straight motion or an orbital revolution depending on the shape of the camphor particle [28].

Another simple artificial realisation of active particle is active liquid droplets, which move due to chemical reactions [33, 34], gradient of the surface tension [35–38], and a polymerisation process [39]. Interestingly, an oil droplet attached by a small piece of solid soap, which is floating on the surface of a water bath, spontaneously exhibits a spinning motion besides a translational straight motion and an orbital revolution [40]. Since a liquid droplet is not rigid but deformable, shape deformation of the particle accompanies its active motion [33, 38].

Another example of active deformable particle is a vesicle, i.e. a closed lipid bilayer, which is often studied as a model biomembrane or a model cell [41]. In some experiments, synthetic vesicles exhibit translational migration [22, 42, 43]. More interestingly, active vesicles even undergo a self-reproduction process [44, 45], which is one of the most important features of living organisms.

To summarise, there are miscellaneous examples of active matter and thus various mechanisms of active motion. Some of them have rigid shape, while the others are soft and deformable, for which deformation of the shape is usually strongly coupled to the particle dynamics. Indeed, for many biological systems, deformability is of basic importance and relevant for their dynamics [46–49]. Due to the existence of internal mechanisms and the couplings of deformations and dynamical movements, single-particle dynamics of active matter are already complicated and provide various challenging physical problems.

A number of elaborated models have been developed for each specific active matter [10, 12, 50–55]. On the other hand, since the active matter includes a wide variety of systems, a basic theoretical description of active matter is needed. One possible way is to consider a possible simple mechanism of active matter [56–58] to clarify the origin of active motion. Besides, it is also required to develop a description that does not depend on any specific internal mechanism relevant to active motions in order to clarify universal dynamics of active matter, in which we actually are interested in this thesis.

³Camphor boat is a toy for kids, where a small piece of camphor solid is attached to the tail of the boat. Camphor dissolves and spreads into the water, and evaporates from the water solution into the air as well. This induces anisotropy of the gradient of camphor concentration between the head and tail of the boat, which gives rise of Marangoni flow. As a result, the camphor boat propels on the surface of the aqueous bath.

Actually, only a camphor solid without boat is enough to propel by itself on a water surface.

1.3 Collective dynamics of active particle

Besides the dynamics of a single active particle, collective dynamics of active matter is a blooming interesting topic. Colloidal active particles are often used to investigate collective dynamics of active matter [3, 4]. There are also a number of studies on the systems of bacterial collective dynamics [1, 5]. On a larger scale, collective active matters include a flock of birds, a school of fish, a herd of animals, and even a crowd of people. Together with the collective system of artificial active particles, this is a well-studied and rapidly spreading field [1, 4, 5, 59–61]. Apart from that, multi particle systems of biological active matter include formation of living organs [62], which actually has received less attention in the field of active matter.

In the case of the multi-particle systems of active matter, increasing numbers of studies have been pushed forward concerning anomalous diffusions [63–67], a long-range ordered state [68–70],⁴ formation of dynamical structures such as traveling bands that appear around the order-disorder transition [72–77], and clustering [78–80], and their rheological properties [81–86]. Interestingly, vertically agitated macroscopic grains have also found the provide some of those properties [87–89]. For these collective dynamics, interactions between particles are of great importance.

In this thesis, however, we do not discuss collective dynamics of active matter. Instead, we consider single-particle dynamics of active matter, to which the existence of internal degrees of freedom is more crucial.

1.4 Active and passive motions

Coming back to a single active particle, active motion, which active particles spontaneously exhibit, is an antonym of passive motion. Passive motion of a particle is what the particle experiences as a direct reaction to external stimuli, or external forces.⁵ In contrast to external force, the force related to active motion is in total zero, i.e. the net force and torque should vanish. This fact is known as *force-free* and *torque-free* properties of active matter. Although active particles are force-free and torque-free, they spontaneously undergo a variety of dynamical motions. Here symmetry breaking plays an important role, as we will see in the next section.

In a similar sense, the term *active Brownian particle* is also used, corresponding to a conventional (passive) Brownian particle [91]. In this context, one of course focuses on stochastic problems, which are usually regarded as extensions of the concepts already

⁴ In active systems, a long-range order has observed even in a two-dimensional space [68–71], where a giant number fluctuation as a result of the rotational symmetry breaking due to the directional movement plays an important role [2].

⁵Therefore the force related to active motions is sometimes referred to as *internal force* and *internal torque* [90]. Although the description in terms of *force* and *torque* for force-free and torque-free active particles seems somewhat strange and contradicts the fact that the net force and torque acting on the particles vanish, it is discussed that the equations of motion of active particles can be mapped onto those of passive particles with shape-dependent grand resistance matrix and formally be external *effective* forces and torques [90].

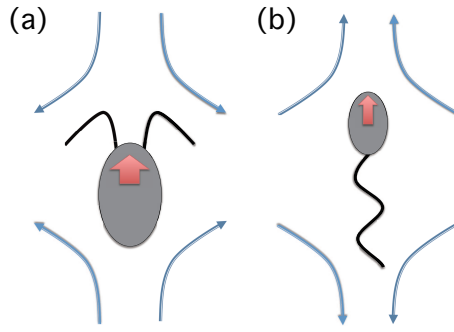


Figure 1.1: Schematic images of (a) a puller and (b) a pusher. The swimmers are propelling in the direction denoted by the red arrows. The blue arrows indicate the flow profile induced by the swimmers (gray circular “bodies” with black “flagella”).

well known in physics such as ordinary Brownian motion. In this thesis, however, we do not put our main focus on the stochastic processes since active particles are already far from equilibrium without stochastic noise. Instead we give a review by Romanczuk *et al.* [91] for more detailed descriptions of active Brownian particles.

1.5 How can active particle move?

An active particle usually is accompanied by various internal degrees of freedom, which are relevant to its spontaneous movements. Therefore, active motion is achieved as a result of cooperative phenomena or dynamical pattern formations of internal statistical processes. The internal degrees of freedom and their dynamical machinery vary for diverse realisation of active matter. This gives a rise to the complexity and difficulty of even the single-particle dynamics of active matter. However, several concepts have been developed to classify active matters.

The translational and rotational motions of active matter are distinguished into two groups depending on where and how they move. One is *crawling* on either solid or soft substrates, and the other is *swimming* in or on the interface of a fluid environment. Crawling is observed for both living cells such as keratocytes [47] and amoebae [8], and artificial active oil droplets [92]. Swimming active matters, or swimmers, such as artificial active colloids and bacteria, are well-studied examples of active matter [1, 4, 5, 52, 59].

Swimmers are further divided into *pusher* and *puller* by the flow profile accompanying the active motion [1, 51, 93]. A pusher, such as bacterium, pushes out the surrounding fluid backward by e.g. flagella, and at the same time forward by head. Therefore the surrounding fluid flows from the side of the pusher to the front and the rear, as schematically shown in Fig. 1.1(b). In contrast, a puller, such as algae including *Chlamydomonas*, pulls the fluid in front of and behind it to its sides. See also Fig. 1.1(a) for a schematic drawing. The concept of puller and pusher becomes rather important when the inter-

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actions with other particles or environment such as confinement are taken into account. That is, the interaction of pullers is attractive in the parallel direction with respect to its centre-of-mass movement, while it is repulsive in the perpendicular direction. On the other hand, pushers have an attractive interaction in the perpendicular direction whereas repulsive in the parallel direction [94].

No matter if it is a puller or a pusher, and no matter if it swims or crawls, an active particle should break some symmetry in order to undergo a spontaneous movement. In the case of swimmers at low Reynolds number, where the inertia does not play a major role, this conception is known as Purcell's Scallop Theorem [95]. In fact, a bacterium has rigid helical flagella combined with rotary molecular motors at the anchor point on the inner cell membrane of the (main) cellular body, and self-propels by rotating the flagella [96]. Spermatozoa, algae, eukaryote have soft flagella or cilia, which have an ability to bend by themselves due to a cytoskeletal structure called axoneme, and can swim by beating them [97–99]. Artificial colloidal particles, which usually have asymmetric surface structures with different chemical or physical properties, induce chemical or thermal gradient around them and as a consequence achieve propulsion by diffusiophoresis, electrophoresis, thermophoresis, or interfacial tension [23, 25].

Asymmetric structure or symmetry breaking is not necessary prescribed from the beginning. In fact, self-propelled liquid droplets or vesicles create asymmetry by itself [38, 43]. Anisotropy of the surface tension of the particle interface, which initially is for instance due to the fluctuation of chemical concentrations around the particle, induces a macroscopic fluid flow called Marangoni flow, which drives the particle. Once the particle moves forward, the spatial symmetry is broken and if the anisotropy of the chemical concentration in the front and the rear is enhanced, it stabilises the asymmetry of the surface tension. As a result, the particle stably propels by itself.

Similarly some living cells such as eukaryote also achieve the asymmetry by itself. In living organisms, various complicated reactions of chemical components and polymerisations of microfilaments such as actin filaments take place. Recently, dynamical observation of the internal chemical reactions and their relationship with morphological changes of the amoeboid shape has been experimentally carried out for *Dictyostelium discoideum* cells [8].

Active motions can also be achieved if the temporal symmetry is not preserved. Najafi and Golestanian studied a simple one-dimensional swimmer in a low Reynolds number fluid, consisting of three rigid spheres connected with two linkers, the lengths of which change between two values periodically [58]. However, this periodic internal motion occurs in a nonreciprocal way, and hence, breaks the time-reversal symmetry. Consequently this swimmer achieves a translational motion at low Reynolds number. Günther and Kruse also investigated a similar simple system [57] by taking into account a more detailed structure of the connecting linkers, where the bifurcation to the translational motion is studied. Besides, Alexander and Yeomans [56] considered a simple model for the propulsion of two interacting dumb-bells.

The temporal symmetry breaking also appears as a time delay. It is known that in reaction-diffusion systems different time scales of chemical components play important roles in the pattern formation such as Turing patterns [100]. The spontaneously formed

patterns are not always static, but can be dynamical. In fact, it is both numerically and analytically performed that the time delay of the activator and inhibitor causes drift instability of an isolated domain in a reaction-diffusion system [101, 102]. In this sense, an isolated dynamical domain in reaction-diffusion system gives another example of active particle. We will discuss this point more in detail in the next section.

1.6 Active particle in reaction-diffusion system

About two decades ago, Krischer and Mikhailov studied the drift bifurcation, or an onset of a translational motion, of a stationary isolated domain (or spot) in a two-dimensional reaction-diffusion system [101]. They considered an activator-inhibitor system described by

$$\frac{du}{dt} = -u + H(u - a) - v + \nabla^2 u \quad (1.1)$$

$$(\epsilon\sigma)^{-1} \frac{dv}{dt} = \mu u - v + \epsilon^{-2} \nabla^2 v, \quad (1.2)$$

where $\epsilon \ll 1$ and σ is an independent parameter. u and v denote activator and inhibitor, respectively, and $H(z)$ is the Heaviside step function, $H(z) = 0$ for $z < 0$ and $H(z) = 1$ for $z > 0$. The parameter a , which represents the excitation threshold of a stable uniform stationary state $u = v = 0$, is assumed to depend on the total activator and inhibitor concentrations in the medium:

$$a = a_0 + \alpha(s - s_0), \quad (1.3)$$

where α is a positive coefficient and

$$s = \int (u + v) d\mathbf{x}. \quad (1.4)$$

Equation (1.3) corresponds to area conservation (volume conservation, in three dimensions) of the excited domain in the limit of $\alpha \rightarrow \infty$. This global coupling is actually crucial for the drift bifurcation of the domain since it prohibits the expansion or shrink of the domain and hence a breathing bifurcation. Indeed, it is discussed that a two-dimensional circular excited domain in two-component reaction-diffusion systems experiences breathing instability or static shape deformations before drift instability [103, 104].

When σ is large, a stationary isolated circular-shaped domain stably exists, while for small σ it experiences a bifurcation to a translating domain and thus starts to migrate with a constant speed [101]. When the domain self-propels, its shape elongates in the vertical direction with respect to the migration direction. The origin of this self-propulsion is understood as follows. Suppose that the activator seeps out of the domain at some point of the boundary. Since the value of the inhibitor is smaller outside of the domain than the inside, the concentration of the activator further increases at the seeping region, provided the increase of the inhibitor, represented by the first term on the right-hand side of Eq. (1.2), is slower. That is, the time scale of the inhibitor is larger than that

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of the activator. Therefore the displacement of the activator is enhanced. At the rear of the domain, on the other hand, the opposite effect occurs; I.e. the activator decreases while the inhibitor keeps almost the same value as before, which further decreases the concentration of the activator at the rear part of the domain. As a result, the domain stably undergoes a translational motion spontaneously.

Several years ago, Ohta *et al.* further analysed Eqs. (1.1) and (1.2) by the interfacial approach, and derived a set of coupled nonlinear time-evolution equations for the centre-of-mass velocity and shape deformation around the drift bifurcation [105, 106]. The formulae of the reduced ordinary differential equations are the same as those we would introduce from symmetry considerations in the next chapter (i.e. Eqs. (2.29)–(2.31)). A similar method was also employed to a three-dimensional fluid-dynamic model of an oil droplet self-propelling in a solvent flow due to Marangoni effect, where a chemical component that occurs as a result of a reaction on the surface of the particle is taken into consideration in addition to a two-component water-oil system [94, 107]. The resulting equations have the same formulae as those obtained from the reaction-diffusion systems.

1.7 Shape of active particle

Active particles take various types of shape, which are not necessarily rigid but are more often deformable and do change in time. The internal structures of active particle and the dynamics of active matter are strongly connected to the shape of the particle. That is, the shape of active matter has non-negligible effect on the particle dynamics. Furthermore, if the particle is deformable and its shape changes dynamically, the particle movement in turn determines the shape of the active matter.

For example, an active colloidal particle, the shape of which is rigid and L-shaped and hence lacking a rotational symmetry, is found to exhibit an orbital revolution in a solution [108]. A C-shaped camphor solid undergoes a straight motion, while, if it has a comma shape, the camphor solid exhibits an orbital revolution [28]. Translational motion of active liquid droplets and active vesicles is accompanied by shape deformations, which strongly couple to their active motion [22, 33, 35, 38, 42, 43]. Active oil droplet attached by a solid soap floating on the interface of aqueous bath even experiences a transition from a straight motion to an orbital revolution spontaneously depending on the size ratio of the oil droplet and the solid soap [40].

For biological organisms, it is rather natural that their movements are strongly related to their shape. Furthermore, the shape of biological organisms is often dynamical, and thus the deformation or the change of shape is of relevant importance for living creatures. On a large scale, i.e. the scale of the living creatures that we can see for instance without microscope such as fish, birds and mammals, it is true obviously and with no doubt. On a nanometre scale, molecular motors and ion pumps work due to the morphological changes by consuming chemical energy of ATP [14, 15]. On an intermediate micrometre scale of a single cell such as eukaryote, it is recently experimentally revealed that the dynamical shape deformation is strongly coupled to the cell movements [46–49].

Despite its practical importance, shape deformation of active matter has been at-

tracted less attention. What we are interested in, however, is active deformable particles, where the deformability of the particle is strongly related to its dynamics. This coupling makes the dynamics of active deformable particles fascinating and complicated. In this thesis, we investigate the dynamics of active deformable particle, where the deformability of the particle shape and the translational and rotational motions are strongly coupled, from a general viewpoint independent of any specific internal mechanism.

1.8 Organisation of this thesis

The organisation of this thesis is as follows. In the next chapter, we consider an active deformable particle in an external flow field. We introduce dynamical degrees of freedom of the active deformable particle, which we take into account in this thesis, namely the position and velocity of the centre of mass, the rotation of the particle, and its shape deformations. The derivation of time-evolution equations for these variables is described, with a review of some of the previous works [109, 110], where the dynamics of an elliptically-deformable self-propelled particle are discussed.

In Chapters 3 and 4, we address the existence of two types of spinning motion for active deformable particles. For simplicity, we consider active deformable particles in a quiescent flow. One is a spinning motion accompanied by the rotation of the whole body, and thus an angular momentum can be defined. This spinning motion is comparable to the spinning motion of a rigid body. We introduce the dynamics of active deformable particles that exhibit this type-I spinning motion as well as a spontaneous translational motion in Chapter 3, which gives a review of Refs. [77, 111, 112].

The other is due to the shape deformations, which translate along the interface as traveling waves. In terms of the dynamics of the particle, these traveling waves of deformations are regarded as a spinning motion. The dynamics of this type-II spinning motion are investigated in Chapter 4, which describes the same results as those of the study of the present author published in Ref. [113].

Chapters 5 and 6 are devoted to the dynamics of active deformable particles in an external flow field. In Chapter 5, a linear shear flow is considered as the simplest example. The results of this chapter are the same as those what the current author published in Ref. [114]. Three types of active particles are distinguished. One is a particle without an active rotation but with only an active translational motion. The others are particles with both active translational and rotational motions, where the direction of the active rotation is on the one hand same as, and on the other hand opposite to that of the passive rotation due to the shear flow.

Moreover, dynamics of active deformable particles in a swirl flow are investigated in Chapter 6. Active deformable particles that tend to elongate in the parallel and perpendicular directions with respect to the direction of the active velocity are found to exhibit different dynamical motions in a swirl. Since the setup of a swirl has a similarity to that of the scattering geometry and thus possesses an analogy to the classical Kepler and Rutherford problems, we numerically perform a similar scattering experiment in terms of active deformable particles. This chapter describes the same results as those in

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Ref. [115].

Chapter 7 is devoted to the summary and conclusions, and the discussion of future problems is as well developed.

Chapter 2

Modelling of active deformable particles from symmetry arguments

In this chapter, we show how to model active soft particles in a systematic way. To this end, one first has to know what degrees of freedom need to be taken into account and how to describe them. Then, coupled time-evolution equations for these variables should be obtained. In the next section, the degrees of freedom of an active deformable particle that we consider in this thesis are introduced. We then discuss the description of the active motion for each degree of freedom in Section 2.2. The couplings among the variables are taken into consideration in Section 2.3, where the dynamics of a deformable self-propelled particle with an elliptical deformation are reviewed. In order to keep the argument general, we describe the variables in tensor form and employ the strategy of symmetry considerations to derive coupled equations of motion. We finally give the summary and conclusions of this chapter in Section 2.4.

2.1 Description of degrees of freedom

A theoretical analysis starts from modelling of the system of interest. In order to model the system, one first has to know what degrees of freedom have to be considered for the analysis. Here, we are interested in the dynamics of an active deformable particle, which requires at least three components; First component is to describe “particle”, the dynamics of which is usually represented by its centre-of-mass position. Second one is for the particle property “deformable”, which is nothing but the deformation of the shape. Finally, for the property “active” we here consider a spontaneous translational motion and a spontaneous rotational motion of the particle. The deformability can also be “active” if the particle changes its shape by itself, which actually plays an important role for various living organisms.

In order to obtain the description of these variables, here we consider an active deformable particle in a flow field. For simplicity, we assume that the flow field is externally imposed and prescribed. The flow velocity $\mathbf{u}$ generally varies in space, and hence, is a given function of space. As usual, two distinct contributions of its spacial derivative are

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treated separately; One is the elongational part of the flow described by the symmetric second-rank tensor $\mathbf{A}$, the (i, j) component of which is defined by

$$A_{ij} = \frac{1}{2} (\partial_i u_j + \partial_j u_i), \quad (2.1)$$

where ∂_i stands for the partial derivative with respect to x_i . The other is the rotational contribution of the flow extracted via the antisymmetric second-rank tensor $\mathbf{W}$, the (i, j) component of which is defined by

$$W_{ij} = \frac{1}{2} (\partial_i u_j - \partial_j u_i). \quad (2.2)$$

Now we consider the variables for the active soft particle. First of all, we denote the centre-of-mass position of the particle at time t as $\mathbf{x}(t)$. The time derivative of the centre-of-mass position, i.e. the total particle velocity, can be divided into two contributions; On the one hand, the particle suffers the *passive* advection due to the surrounding flow field $\mathbf{u}$. On the other hand, the particle can self-propel in an *active* manner with respect to the surrounding flow field. The *active* velocity measured with respect to the surrounding flow velocity is denoted by $\mathbf{v}$. Altogether, the equation of motion for the centre of mass position is given by

$$\frac{dx_i}{dt} = u_i + v_i, \quad (2.3)$$

where the index i labels the Cartesian coordinates. In our description, the active velocity $\mathbf{v}$ is one of our major dynamical variables, describing the self-propelling behavior of the active particle.

Another important dynamical variable is the rotation of the whole particle around its centre of mass. Indeed some active particles spontaneously experience rotation around its centre of mass [40, 116–121]. Besides the rotation that the active particle spontaneously exhibits, the particle can already be *passively* rotated by the surrounding flow field $\mathbf{u}$, which is described by an antisymmetric tensor $\mathbf{W}$ given by Eq. (2.2). Therefore, in the same way as for the total velocity of the centre of mass above, the rotation of the particle can be separated into these two contributions. In other words, we can naturally introduce an antisymmetric tensor $\mathbf{\Omega}$ to represent the relative rotation with respect to the rotation $\mathbf{W}$ due to the surrounding flow. We refer to this rotation of the particle $\mathbf{\Omega}$ as active rotation or internal rotation. The antisymmetric tensor $\mathbf{\Omega}$ is related to the (active) angular velocity $\boldsymbol{\omega}$ via

$$\Omega_{ij} = \epsilon_{ijk} \omega_k. \quad (2.4)$$

where ϵ_{ijk} stands for the (i, j, k) component of the Levi-Civita tensor. Summation over the repeated indices is implied throughout this thesis. Consequently, antisymmetric tensor $\mathbf{W} + \mathbf{\Omega}$ describes the total angular velocity of the particle measured from the laboratory frame, from which the flow field is parameterized.¹

¹ In order to “see” the rotation of a circular particle (a spherical particle in three dimensions), one needs to follow a marker point on the particle $\mathbf{p}$, the time evolution of which is governed by

$$\frac{dp_i}{dt} = -(W_{ij} + \Omega_{ij}) p_j. \quad (2.5)$$

Finally, we introduce variables for the deformation of the particle. Since deformation of a particle is the change of its shape from the original steady shape, it is sufficient to consider the deviation of the interface of the particle. Here we only consider a two-dimensional case,² where orientations on the two-dimensional plane can be parameterized by a single angle θ . This angle θ is used to measure directions around the particle centre of mass. We describe the distance from the centre of mass to the interface of the particle in the direction θ at time t by the local radius $R(\theta, t)$. Here, a large deformation is not taken into account so that $R(\theta, t)$ is single-valued with respect to the angle θ . We assume that the original steady shape is a circle, i.e. $R(\theta, t) = R_0$ with the radius R_0 a given constant. Then, the local radius $R(\theta, t)$ can be divided into two parts;

$$R(\theta, t) = R_0 + \delta R(\theta, t), \quad (2.6)$$

where δR is (small) deviation from the original steady shape. The deviation from the steady circular shape is expanded into Fourier series

$$\begin{aligned} \delta R(\theta, t) &= \sum_{m=2}^{\infty} \left(z_m(t) e^{im\theta} + z_{-m}(t) e^{-im\theta} \right) \\ &= \sum_{m=2}^{\infty} 2A_m(t) \cos m(\theta - \theta_m), \end{aligned} \quad (2.7)$$

where we have defined

$$z_m = A_m(t) e^{-im\theta_m}. \quad (2.8)$$

A_m and θ_m correspond to the magnitude and the direction of the deformation, respectively. Since the local radius $R(\theta, t)$ is a real variable, $A_m = A_{-m}$ is required. Here, the zeroth mode can be excluded by assuming that the area of the particle is conserved, which is the case we consider in this thesis. The first-order Fourier mode actually represents the translation of the centre of mass, which we have already taken into account by the active velocity $\mathbf{v}$. Therefore the lowest mode of deformation is the second mode, which represents an elliptical deformation.

The Fourier coefficients of deformation can be transformed into symmetric tensor variables. Symmetric tensors in a three-dimensional space have been formulated in Ref. [122]. Here we formulate symmetric tensors in a two-dimensional space.³ First of all, we note that a symmetric tensor of order n has n mirror-symmetry axes, the m th unitary vector of which ($m = 0, 1, \dots, n-1$) is given by

$$\mathbf{N}^{(n,m)} = \left(\cos \left(\theta_n + \frac{2m}{n} \pi \right), \sin \left(\theta_n + \frac{2m}{n} \pi \right) \right). \quad (2.9)$$

² The deformation in a three-dimensional space can also be taken into account in the same manner. In this case, however, the deviation of the local radius should be expanded in terms of spherical harmonics. The description by the symmetric deformation tensors is still valid in three dimensions, which can be related to the coefficients of the spherical harmonic expansion.

³ Note that the definition of the symmetric deformation tensors is independent of the Fourier expansion (and the expansion with spherical harmonics in three dimensions) of the local radius. Therefore, the description with the symmetric deformation tensors gives a general and systematic formulation that is valid for both two and three dimensions.

2 Modelling of active deformable particles from symmetry arguments

In the case of $n = 2$, the (i, j) component of a second-order traceless symmetric tensor $\mathbf{S}$ is defined from the symmetry axes, Eq. (2.9) with $n = 2$, as⁴

$$S_{ij} = \delta_2 \sum_{m=0,1} \left(N_i^{(2,m)} N_j^{(2,m)} - \frac{1}{2} \delta_{ij} \right). \quad (2.10)$$

From Eq. (2.10), the relation between the symmetric tensor $\mathbf{S}$ and the second-order Fourier mode is given by

$$S_{11} = -S_{22} = s_2 \cos 2\theta_2 = z_2 + z_{-2} \quad (2.11)$$

$$S_{12} = S_{21} = s_2 \sin 2\theta_2 = i(z_2 - z_{-2}), \quad (2.12)$$

where we have written $s_2 = 2A_2 = \delta_2$. In the same way, the third-order symmetric tensor is defined from Eq. (2.9) with $n = 3$ by

$$U_{ijk} = \delta_3 \sum_{m=0,1,2} N_i^{(3,m)} N_j^{(3,m)} N_k^{(3,m)}. \quad (2.13)$$

Then, the third-order Fourier mode, which represents a triangular deformation, can be transformed into a third-order symmetric tensor $\mathbf{U}$ by

$$U_{111} = -U_{122} = -U_{212} = -U_{221} = s_3 \cos 3\theta_3 = z_3 + z_{-3} \quad (2.14)$$

$$U_{112} = U_{121} = U_{211} = -U_{222} = s_3 \sin 3\theta_3 = i(z_3 - z_{-3}), \quad (2.15)$$

where $s_3 = 2A_3 = (3/4)\delta_3$. Finally, a symmetric tensor of fourth order is given from Eq. (2.9) with $n = 4$ by

$$T_{ijkl} = \delta_4 \sum_{m=0}^3 \left\{ N_i^{(4,m)} N_j^{(4,m)} N_k^{(4,m)} N_l^{(4,m)} - \frac{1}{8} (\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \right\}. \quad (2.16)$$

The fourth-order Fourier mode representing a quadratic deformation, which actually is the highest mode deformation that we deal with in this thesis, is related to a fourth-order symmetric tensor $\mathbf{T}$ by

$$T_{1111} = T_{2222} = -T_{1122} = s_4 \cos 4\theta_4 = z_4 + z_{-4} \quad (2.17)$$

$$T_{1112} = -T_{1222} = s_4 \sin 4\theta_4 = i(z_4 - z_{-4}), \quad (2.18)$$

where $s_4 = 2A_4 = \delta_4/2$. The other components are obtained by the symmetric property of the tensor $\mathbf{T}$ as

$$\begin{aligned} T_{1122} &= T_{1221} = T_{1212} = T_{2112} = T_{2121} = T_{2211}, \\ T_{1112} &= T_{1121} = T_{1211} = T_{2111} = -T_{1222} = -T_{2122} = -T_{2212} = -T_{2221}. \end{aligned} \quad (2.19)$$

In general, n th-order Fourier mode deformation can be related to and described by a symmetric tensor of order n , $\mathbf{M}^{(n)}$.

⁴ The traceless property is required to eliminate the contribution of the zeroth mode.

Using these symmetric tensor expressions of the deformations, the local radius in Eq. (2.6) is rewritten as⁵

$$R(\theta, t) = R_0 + S_{11} \cos 2\theta + S_{12} \sin 2\theta + U_{111} \cos 3\theta + U_{112} \sin 3\theta \\ + T_{1111} \cos 4\theta + T_{1112} \sin 4\theta + \dots \quad (2.21)$$

In this way, we can deal with the deformation of the particle systematically. This strategy is also applicable to a three-dimensional case, where the shape deformation should be expanded in terms of spherical harmonics.

2.2 Equations for active motions

In the previous section, we obtained the variables of an active deformable particle: the active velocity of the centre of mass as a vector variable $\mathbf{v}$, the active rotation as a second-rank antisymmetric tensor variable Ω , and the n th-mode deformation as n th-order symmetric tensor variables $\mathbf{M}^{(n)}$. In this and the next sections, we show how to introduce time-evolution equations for these variables. We first consider how to derive the equations to represent active motion in this section. Then, the couplings among the variables will be discussed in the next section. To keep the argument general, we employ the strategy of symmetry considerations.

In this section, we investigate the expressions for spontaneous motion of the particle. There are several types of spontaneous motions that an active particle exhibits. For generality, we employ the bifurcation theorem so that it is not necessary to specify any mechanism of the active motion. To this end, we here assume a bifurcation of the supercritical pitchfork type. The normal form of supercritical bifurcation is described as

$$\frac{d\psi}{dt} = \tau\psi - \psi^3. \quad (2.22)$$

Equation (2.22) has a trivial solution $\psi = 0$, which is stable as long as τ is negative. When τ crosses 0 and becomes positive, this solution suffers instability and a pair of steady solutions $\psi = \pm\sqrt{\tau}$ appear to be stable. See Fig. 2.1.

Now we consider the self-propulsion of an active particle. In the field of nonlinear dynamics, this is known as a drift bifurcation. Here we assume that the drift bifurcation

⁵ There is another possibility to define a deformed shape by using the deformation tensors:

$$\tilde{\mathbf{r}}_i = \|\mathbf{r}\| (n_i + S_{ij}n_j + U_{ijk}n_jn_k + T_{ijkl}n_jn_kn_l + \dots) \quad (2.20)$$

where $\mathbf{r} \equiv \|\mathbf{r}\|\mathbf{n}$ represents the position of the interface of the undeformed shape, and $\tilde{\mathbf{r}}$ is that of the deformed shape. Here note that, from the relation (2.20), $\|\tilde{\mathbf{r}}\| \neq \|\mathbf{r}\|$ and $\tilde{\mathbf{r}}/\|\tilde{\mathbf{r}}\| \neq \mathbf{r}/\|\mathbf{r}\| = \mathbf{n}$. The two expressions, Eqs. (2.20) and (2.21), coincide up to the first order of the deformations, i.e. $O(\delta_m\delta_n)$.

One may start the argument of the definition of the particle deformation from Eq. (2.20) with symmetric deformation tensors defined by Eqs. (2.10), (2.13) and (2.16). In this case, it is not necessary to consider the relation of the symmetric tensors and the Fourier components of the deviation of the local radius. Still, the dynamics governed by the coupled time-evolution equations of the deformation tensors that we develop in this thesis remains the same but only the visualisation of the resulting deformation and hence the particle shape changes slightly.

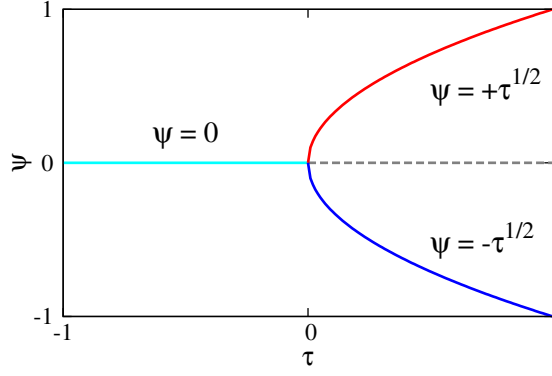


Figure 2.1: Solutions of Eq. (2.22) around a supercritical pitchfork bifurcation. Solid and dashed lines represent stable and unstable solutions, respectively.

is of the supercritical pitchfork type. Then, from Eq. (2.22), the self-propulsion of the active particle is described as

$$\frac{dv_i}{dt} = -\kappa_1 v_i - (v_k v_k) v_i. \quad (2.23)$$

First term on the right-hand side of Eq. (2.23) is a usual form of a friction term if $\kappa_1 > 0$, and hence, represents the energy dissipation. As a result, no drift occurs for $\kappa_1 > 0$. When κ_1 becomes negative, however, this term gives an inverse friction and works as energy input to the particle. Therefore balancing with the cubic term in the second term on the right hand side of Eq. (2.23) representing the energy dissipation, the particle acquires a spontaneous velocity $|v| = \sqrt{-\kappa_1}$. The direction of the motion depends on the initial condition. Again, we emphasise that, with this expression, we do not need to specify any detailed propulsion mechanism. In this manner, we obtain a general description of equation of motion for active propulsion around the drift bifurcation.

In the same way, the equation of motion for the active rotation reads

$$\frac{d\Omega_{ij}}{dt} = \zeta \Omega_{ij} - (\Omega_{k\ell} \Omega_{k\ell}) \Omega_{ij}. \quad (2.24)$$

In two dimensions, the antisymmetric tensor Ω is given by

$$\Omega = \begin{bmatrix} 0 & \omega \\ -\omega & 0 \end{bmatrix}, \quad (2.25)$$

with which Eq. (2.24) is rewritten as

$$\frac{d\omega}{dt} = \zeta \omega - 2\omega^3. \quad (2.26)$$

For $\zeta < 0$, only the trivial solution $\omega = 0$ exists, while a pair of solutions $\omega = \pm\sqrt{\zeta}$ appear for $\zeta > 0$. The different signs of the pair of the latter solutions correspond to the rotation in the counter-clockwise and clockwise direction, respectively.

2.3 Couplings between velocity and deformation

Finally, in the case that the deformation appears spontaneously, we again describe it in the form of the supercritical pitchfork bifurcation. For example, for the elliptical second mode deformation S , the equation of motion is written from Eq. (2.22) as

$$\frac{dS_{ij}}{dt} = -\kappa_2 S_{ij} - (S_{k\ell} S_{k\ell}) S_{ij}, \quad (2.27)$$

where κ_2 represents the stiffness of the particle if it is positive, but it characterise the magnitude of the elliptical deformation if $\kappa_2 < 0$. In general, n th mode deformation $M^{(n)}$ that occurs spontaneously obeys the following equation of motion;

$$\frac{dM_{\mathbf{i}}^{(n)}}{dt} = -\kappa_n M_{\mathbf{i}}^{(n)} - \left(M_{\mathbf{j}}^{(n)} M_{\mathbf{j}}^{(n)} \right) M_{\mathbf{i}}^{(n)}, \quad (2.28)$$

where the indices $\mathbf{i}$ and $\mathbf{j}$ denote index vectors of dimension n .

2.3 Couplings between velocity and deformation

We finally introduce nonlinear couplings among the variables. In this thesis, we achieve it by the strategy of symmetry considerations. Generally speaking, the equations of motion should satisfy translational and rotational symmetries unless these symmetries are broken due to external fields. In other words, the time evolution equations should recover those symmetries when the external fields are switched off. In the following, we show an example considering a deformable self-propelled particle in a quiescent environment and take into account couplings among the velocity and shape deformation. For simplicity we take into consideration the active translational motion and the elliptical deformation. This is a review of the previous works in Ref. [109, 110].

2.3.1 Self-propelled particle with elliptical deformation

Here we consider a deformable self-propelled particle with an elliptical deformation S in a quiescent environment. From symmetry considerations, time-evolution equations read

$$\frac{dx_i}{dt} = v_i, \quad (2.29)$$

$$\frac{dv_i}{dt} = -\kappa_1 v_i - a_0 (v_\ell v_\ell) v_i - a_1 S_{i\ell} v_\ell, \quad (2.30)$$

$$\frac{dS_{ij}}{dt} = -\kappa_2 S_{ij} - b_0 (S_{\ell m} S_{\ell m}) S_{ij} + b_1 \left[v_i v_j - \frac{v_\ell v_\ell}{2} \delta_{ij} \right]. \quad (2.31)$$

The couplings of the velocity and deformation are taken into consideration to the lowest order. If the coefficients a_1 and b_1 have different signs, i.e. $a_1 b_1 < 0$, Eqs. (2.29)–(2.31) are variational, which is not the case we consider in this thesis. Instead, here we concentrate on the dissipative case, i.e. $a_1 b_1 > 0$. We note that the coupled equations (2.29)–(2.31) is symmetric against the simultaneous transformation: $S_{ij} \rightarrow -S_{ij}$ and $(a_1, b_1) \rightarrow (-a_1, -b_1)$. This set of time-evolution equations has originally been investigated in

2 Modelling of active deformable particles from symmetry arguments

Refs. [109, 110]. In the following, we briefly review the dynamics obtained from the set of equations (2.29)–(2.31).⁶

When the particle deformation does not occur spontaneously, i.e., $\kappa_2 > 0$, one does not need to consider the higher-order relaxation term and hence, may put $b_0 = 0$ in Eq. (2.31). The dynamics obeying Eqs. (2.29)–(2.31) is determined by $\mathbf{v}$ and $\mathbf{S}$ and thus we have Eqs. (2.30) and (2.31) to consider. Describing the velocity and the elliptical deformation with magnitudes and characteristic angles as

$$\mathbf{v} = (v \cos \phi, v \sin \phi), \quad (2.32)$$

$$S_{11} = -S_{22} = s \cos 2\theta_2, \quad S_{12} = S_{21} = s \sin 2\theta_2, \quad (2.33)$$

Eqs. (2.30) and (2.31) become

$$\frac{dv}{dt} = -\kappa_1 v - a_0 v^3 - a_1 v s \cos 2\psi, \quad (2.34)$$

$$\frac{d\phi}{dt} = -a_1 s \sin 2\psi, \quad (2.35)$$

$$\frac{ds}{dt} = -\kappa_2 s + \frac{b_1}{2} v^2 \cos 2\psi, \quad (2.36)$$

$$\frac{d\theta_2}{dt} = -\frac{b_1 v^2}{4s} \sin 2\psi, \quad (2.37)$$

where we have defined the relative angle $\psi = \theta_2 - \phi$. From Eqs. (2.34)–(2.37), the time evolution is determined by v , s , and ψ . Therefore, the equations of motion that we have to consider is Eqs. (2.34) and (2.36) as well as

$$\frac{d\psi}{dt} = \left(-\frac{b_1 v^2}{4s} + a_1 s \right) \sin 2\psi. \quad (2.38)$$

The set of Eqs. (2.34) and (2.36) have one trivial solution $(v, s) = (0, 0)$ and one nontrivial solution

$$v = \left(\frac{-\kappa_1}{a_0 + B \cos^2 2\psi} \right)^{1/2}, \quad s = \frac{-\kappa_1 B \cos 2\psi}{a_1(a_0 + B \cos^2 2\psi)}, \quad (2.39)$$

where we have written

$$B = \frac{a_1 b_1}{2\kappa_2}. \quad (2.40)$$

For the trivial solution, the angles ϕ and θ_2 lose their meaning, so does their relative angle ψ . Therefore, we do not consider the angle ψ for this solution, which indeed does not affect the stability of this trivial solution. From a usual stability analysis, the stability condition of the trivial solution is obtained as $\kappa_1 < 0$ [109, 110].

⁶ We newly carried out the numerical simulations in this section.

2.3 Couplings between velocity and deformation

On the other hand, for the nontrivial solutions given by Eq. (2.39), Eq. (2.38) is rewritten as

$$\frac{d\psi}{dt} = \left(-\frac{\kappa_2}{2 \cos 2\psi} + \frac{-\kappa_1 B \cos 2\psi}{a_0 + B \cos^2 2\psi} \right) \sin 2\psi \quad (2.41)$$

$$= -\frac{\kappa_2 a_0 + 2B(\kappa_2 + \kappa_1) \cos^2 2\psi}{2(a_0 + B \cos^2 2\psi)} \tan 2\psi, \quad (2.42)$$

which has two solutions [109, 110]. One is $\sin 2\psi = 0$, and the other is given by

$$\cos^2 2\psi = \frac{\kappa_2 a_0}{2B(-\kappa_1 - \kappa_2)}. \quad (2.43)$$

The sign of $\cos 2\psi$ must be determined to satisfy the condition $s > 0$ in Eq. (2.39). That is, it takes positive sign for $a_1 > 0$ and negative for $a_1 < 0$. Here, note that the right-hand side of Eq. (2.43) must be non-negative and thus $B > 0$ in Eq. (2.40). Since $\cos^2 2\psi \leq 1$, this solution exists as long as

$$\kappa_1 \leq \kappa_1^c \equiv -\frac{a_0 + 2B}{2B} \kappa_2. \quad (2.44)$$

A usual linear stability analysis reveals that the solution $\sin 2\psi = 0$ is stable as long as $\kappa_1^c \leq \kappa_1 \leq 0$ while the stability condition of the solution obtained as Eq. (2.43) is $\kappa_1 \leq \kappa_1^c$.

As a result, Eqs. (2.30) and (2.31) have three types of solutions [109, 110]. One is a trivial solution, i.e., $\mathbf{v} = \mathbf{0}$ and $\mathbf{S} = \mathbf{0}$, where the particle is motionless with a circular shape without deformation. The motionless state is stable for $\kappa_1 > 0$. For $\kappa_1 < 0$, the trivial solution becomes unstable and the particle starts to undergo a straight motion [109, 110]. The solution of the straight state is described by Eq. (2.39) and $\sin 2\psi = 0$ and is stable as long as $\kappa_1^c \leq \kappa_1 \leq 0$. The direction of the motion in real space is determined by the initial condition. In contrast, for $\kappa_1 \leq \kappa_1^c$, the set of the solutions given by Eqs. (2.39) and (2.43) represents a circular state, that is, the particle undergoes a translational motion in a closed circular trajectory.

Now we show the results obtained by numerically solving the time-evolution equations (2.29)–(2.31) for varying κ_1 and κ_2 with the other parameters fixed as $a_0 = 1 = b_0$ and $a_1 = -1.5 = b_1$. We let both κ_1 and κ_2 take positive and negative values, and thus the elliptical deformation $\mathbf{S}$ in addition to the centre-of-mass velocity $\mathbf{v}$ may occur spontaneously. The results are summarised in Fig. 2.2, where we show the dynamical phase diagram in the panel (a) and some examples of the particle silhouettes and trajectories of the particle for the dynamical states in the panels (b)–(i). The size of the silhouette is adjusted for illustration though the radius of the original circular shape is always set to unity, $R_0 = 1$. In Fig. 2.2(a), all but one of the bifurcation boundaries are superposed, which are obtained analytically. Here we do not show the details of the analytical formulae and their derivation since it can be carried out in a straightforward way and, from the mathematical symmetry of the time-evolution equations as will be discussed in Section 4.2 of Chapter 4, it is calculated in the almost same way as those in Section 4.3 of Chapter 4.

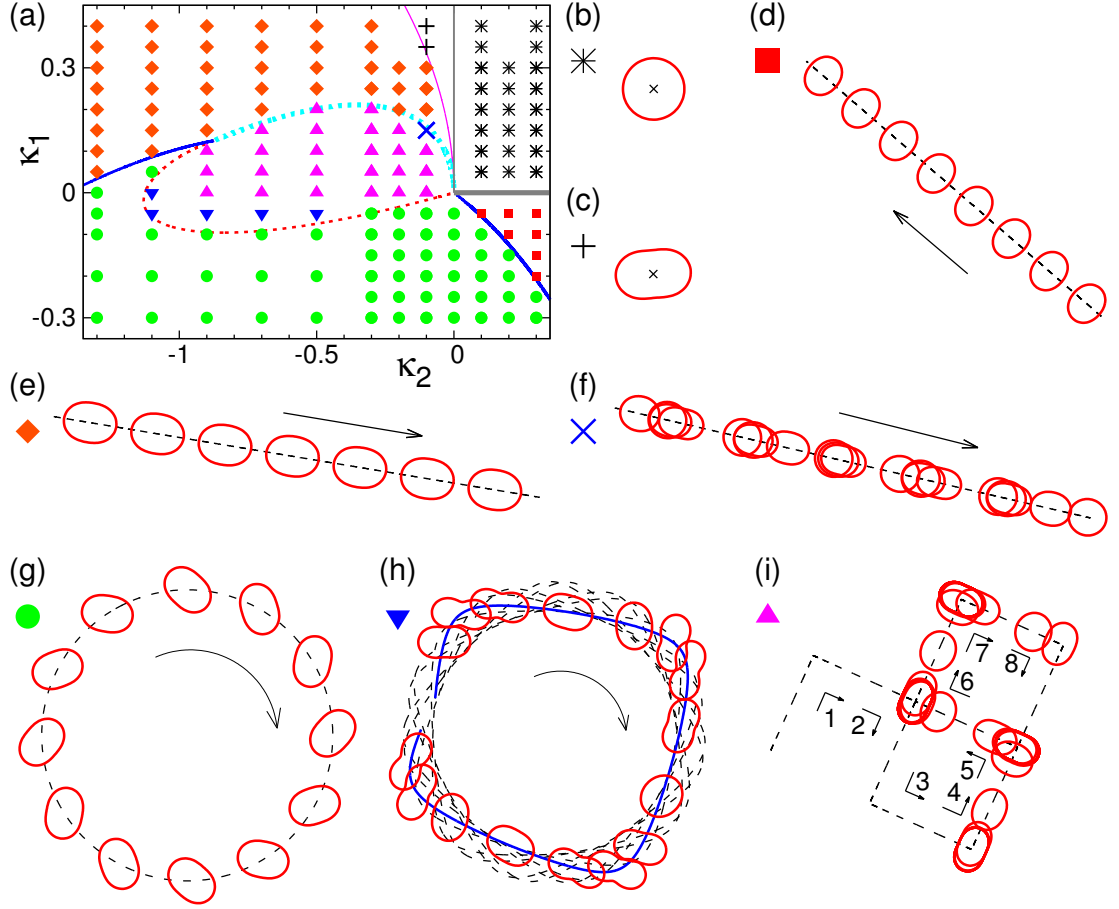


Figure 2.2: (a) Phase diagram of an elliptically-deformable active particle. The solid and dashed lines show the boundaries of supercritical pitchfork bifurcations and Hopf bifurcations, respectively, which are obtained analytically. (b) and (c) Silhouettes of the particles at (b) the motionless state for $\kappa_1 = 0.1$ and $\kappa_2 = 0.1$ and (c) the static elliptical-deformation state for $\kappa_1 = 0.4$ and $\kappa_2 = -0.1$. The crosses indicate the position of the centre of mass, which is motionless. (d)–(i) Trajectories of the centre of mass of (d) the straight I state for $\kappa_1 = -0.2$ and $\kappa_2 = 0.3$; (e) the straight II state for $\kappa_1 = 0.2$ and $\kappa_2 = -0.1$; (f) the oscillatory straight state for $\kappa_1 = 0.15$ and $\kappa_2 = -0.1$; (g) the circular state for $\kappa_1 = -0.1$ and $\kappa_2 = -0.1$; (h) the quasi-periodic state for $\kappa_1 = -0.05$ and $\kappa_2 = -0.5$; and (i) the rectangular state for $\kappa_1 = 0.05$ and $\kappa_2 = -0.1$. Some silhouettes of the particle are superposed, the size of which is adjusted for illustration. The symbols in the panels (b)–(i) correspond to those in the diagram in the panel (a). In the panel (h), trajectory for short time interval is emphasised by the blue solid line. The arrows in the panels (d)–(i) indicate the direction of motion. Numbers in the panel (i) represent the chronological order. These are obtained by solving the coupled equations (2.30)–(2.31) numerically for $a_0 = b_0 = 1$ and $a_1 = b_1 = -1.5$.

2.3 Couplings between velocity and deformation

As mentioned above, Eqs. (2.29)–(2.31) have a trivial solution $(\mathbf{v}, \mathbf{S}) = (\mathbf{0}, \mathbf{0})$. This solution corresponds to a circular-shaped particle without deformation with its centre of mass motionless, as shown in Fig. 2.2(b) for $\kappa_1 = 0.1$ and $\kappa_2 = 0.1$. We call it a motionless state in this thesis. This motionless state is stable as long as $\kappa_1 > 0$ and $\kappa_2 > 0$, as plotted by the black stars in Fig. 2.2(a).

The motionless state loses its stability in two different ways, both of which are bifurcation of supercritical pitchfork type. On the one hand, when κ_1 decreases, the velocity $\mathbf{v}$ experiences a bifurcation at $\kappa_1 = 0$ and the particle starts to migrate spontaneously for $\kappa_1 < 0$. The centre of mass of the particle of this solution draws a straight trajectory, the direction of which is determined by the initial condition. Though the coupling, i.e. the last term on the right-hand side of Eq. (2.31), this finite velocity induces an elliptical deformation, as shown in Fig. 2.2(d) for $\kappa_1 = -0.2$ and $\kappa_2 = 0.3$. We name this motion a straight I motion in this thesis. The parameter region of this straight I motion is plotted by the red filled square in Fig. 2.2(a). Here, note that the particle elongates in the perpendicular direction to the migration direction. Further decreasing κ_1 , this straight I motion suffers instability, where it loses stability in the lateral direction with respect to the migration. As a result, the particle undergoes a circular motion, a trajectory of which in real space is depicted in Fig. 2.2(g) for $\kappa_1 = -0.1$ and $\kappa_2 = -0.1$. The region where the circular motion occurs is plotted by the green filled circles in Fig. 2.2(a). The circular motion dominates the phase diagram for small κ_1 .

On the other hand, if one decreases κ_2 from the motionless state, this time the deformation tensor $\mathbf{S}$ experiences a bifurcation at $\kappa_2 = 0$ and an elliptical deformation takes place for $\kappa_2 < 0$. After the elliptical deformation appears, there still is a finite region where the centre of mass of the particle is motionless as shown by the plus symbols in Fig. 2.2(a). In this region, a motionless particle with static elliptical deformation is observed, as displayed in Fig. 2.2(c) for $\kappa_1 = 0.4$ and $\kappa_2 = -0.1$. Further decreasing κ_2 , the elliptical particle starts to undergo a migration, the centre of mass of which draws a straight trajectory as depicted in Fig. 2.2(e) for $\kappa_1 = 0.2$ and $\kappa_2 = -0.1$. Note that the direction of the deformation of this straight motion is different from that of the above straight I motion in Fig. 2.2(d). The elongation direction is parallel to the migration direction for this straight motion, while it is perpendicular for the straight I motion. Therefore, we name this straight motion as a straight II motion to distinguish from the straight I motion. The region where this straight II motion occurs is plotted by the vermilion filled diamond symbol in Fig. 2.2(a).

Now we decrease κ_1 starting from the straight II motion, which experiences two types of instability depending on the parameter. For small κ_2 , the straight II motion becomes unstable by a supercritical pitchfork bifurcation and the circular motion appears after the bifurcation, as displayed by the green filled circles in Fig. 2.2(a). For large but negative κ_2 , on the other hand, the straight II motion loses its stability by a Hopf bifurcation. In general, one may expect an oscillatory behaviour after a Hopf bifurcation. In this case, it is actually an oscillation of the magnitudes of the velocity and the elliptical deformation. As a result, the particle undergoes an oscillatory straight motion, as depicted in Fig. 2.2(f) for $\kappa_1 = 0.15$ and $\kappa_2 = -0.1$. This oscillatory straight motion was unfortunately not reported in the previous work [109]. The reason may be that the region

where the oscillatory straight motion occurs is extremely narrow in the phase diagram. Indeed, in Fig. 2.2(a), it is only one point denoted by the blue cross symbol. We however observed the oscillatory straight motion at more different parameters although we do not include them in Fig. 2.2(a) since they are too close to the Hopf bifurcation.⁷ Soon after the oscillatory straight motion appears, it is taken its place by a rectangular motion, the trajectory of which is displayed in Fig. 2.2(i) for $\kappa_1 = 0.05$ and $\kappa_2 = -0.1$. The turning angle is $\pi/2$ but its direction, i.e. whether it turns right or left, is determined in a stochastic manner or by a numerical error of the simulation, as indicated by the chronological order 1–8 in Fig. 2.2(i). The particle spends most of the time staying at the turning region and less time for the migration. The parameter region of the rectangular motion is plotted by the purple up triangles in Fig. 2.2(a). Further decreasing κ_2 , another dynamical motion appears before the circular motion dominates the diagram. It is a quasi-periodic motion, as shown in Fig. 2.2(h) for $\kappa_1 = -0.05$ and $\kappa_2 = -0.5$. The quasi-periodic motion is obtained at the blue down triangles in Fig. 2.2(a).

2.4 Summary and conclusions

To summarise this chapter, we introduced the variables that we will use in the rest of this thesis. Considering an active deformable particle in an external flow field, degrees of freedom that we have to take into account are the centre-of-mass position and velocity, the rotation of the particle, and the deformation of the particle shape.

The flow field is represented by flow velocity $\mathbf{u}$, which generally is a function of space. The spatial dependence of the flow velocity is given by the derivative of the flow velocity with respect to the spatial variable, $\partial_i u_j$. As usual, the spatial derivative of the flow velocity is divided into two contributions; Namely, the symmetric part representing the elongational contribution $A_{ij} = (\partial_i u_j + \partial_j u_i)/2$ and the rotational contribution given by the antisymmetric tensor $W_{ij} = (\partial_i u_j - \partial_j u_i)/2$.

The time evolution of the centre-of-mass position $\mathbf{x}$, i.e. the centre-of-mass velocity, consists of two parts: one is the velocity of the flow field $\mathbf{u}$ and the other is the relative velocity $\mathbf{v}$ with respect to it. The origin of this relative velocity is the spontaneous translational motion of the active particle. In the same way, the rotation of the particle is also described by the superposition of the rotation due to the external flow $\mathbf{W}$ and the relative rotation $\mathbf{\Omega}$, which comes from the active rotation, with respect to $\mathbf{W}$. Since the rotational contribution of flow is given by an antisymmetric tensor, the active rotation is also described by an antisymmetric tensor variable.

Finally, we described the deformation of the particle by using symmetric deformation tensors. This expression enables us to include deformation into the equation of motion of a deformable particle in a systematic way. Symmetric deformation tensor of n th order can be related to n th-order Fourier mode of deformation in a two-dimensional space.

For these variables, we derived the equations of motion by symmetry considerations. That is, the description of system should satisfy the translational and rotational sym-

⁷ We further checked that the region where the oscillatory straight motion appears expands for different parameters.

metries. The active motion, which results from a property of the system far from equilibrium as discussed in the previous chapter, is related to the spontaneous breaking of the corresponding symmetry. Therefore, we described it by a Ginzburg-Landau type equation as in Eq. (2.22). Here we assumed each active motion occurs via a supercritical pitchfork bifurcation. The couplings among the dynamical variables are also derived from symmetry considerations.

In addition, the dynamics of a self-propelled particle with an elliptical deformation were reviewed as an example [109, 110]. The time-evolution equations are given by Eqs. (2.29)–(2.31). The results are summarised in Fig. 2.2. It has been known [109, 110] that the active deformable particle experiences a bifurcation from a straight motion to a circular motion due to the coupling between the self-propulsion and the shape deformation. When the particle deformation occurs spontaneously, there is another bifurcation from a circular motion to a quasi-periodic motion [109]. Between the quasi-periodic motion and the straight motion, a rectangular motion appears [109]. In this thesis, we reported another type of dynamical motion, which has been overlooked in the previous work [109]. That is an oscillatory straight motion, where the particle undergoes a translational motion in a straight line with its speed oscillating in time, as shown in Fig. 2.2(f). The bifurcation lines are also obtained analytically.

In conclusion, we briefly comment on the derivation of the time-evolution equations, Eqs. (2.29)–(2.31), from continuous models. So far two continuous models have been reduced to Eqs. (2.29)–(2.31). One is a two-component reaction-diffusion equation with a global coupling, where an isolated domain structure appears spontaneously. In Ref. [101], they reported that an isolated domain experiences a drift bifurcation and exhibits a translational motion. Ohta *et al.* have reduced the partial-differential equations to a set of ordinary-differential equations by an interfacial approach [102, 105]. Another derivation has recently been developed [94, 107] from a continuous model of a droplet in a Stokesian fluid solution, where a chemical reaction takes place on the interface of the droplet. Interestingly, in these cases, there is a tendency that the particle deforms in a perpendicular direction with respect to the active velocity. These studies imply possible realisations and the validity of the model, Eqs. (2.29)–(2.31), which is derived from symmetry considerations.

Chapter 3

Two types of spinning motion

Among active motions, there are two basic dynamical motions. One is a spontaneous translational motion of the centre of mass, i.e. an active migration. The other is an active spinning motion, i.e. spontaneous rotation of the particle around its centre of mass. In fact, there are many experiments of active soft artificial particles and living organisms that undergo a spinning motion spontaneously [8, 40, 49, 116–121, 123, 124].

In this and the next chapters, we concentrate on the spinning motion of active deformable particles. In particular, we argue that, if a particle is deformable, there are at least two types of spinning motion. On the one hand, a particle spins due to the rotation of the whole body. We refer to this type of spinning motion as a type-I spinning motion in this thesis. For the type-I spinning motion, an angular momentum can be defined in the same procedure as for a classical rigid body [125, 126].

On the other hand, if a particle is deformable, the deformation is not always static, but can be dynamical and can change in time. In this case, there is a possibility that the deformation travels along the interface of the particle. Indeed, in some experimental studies, a spinning motion of an active soft object is related to a chemical wave inside the particle [8] or traveling waves on the interface [49, 123, 124]. This *traveling wave* of deformation along the interface appears as a spinning motion in terms of the particle dynamics, which we call a type-II spinning motion in this thesis. In this case, the interfacial motion plays an important role and the whole body of the particle does not necessarily rotate.

The aim of this and the next chapters is to introduce and study theoretical models for these two types of spinning motion of active deformable particles. To keep the argument simple and clear, we consider an active deformable particle in a quiescent environment.

In this chapter, we discuss the dynamics of active deformable particles that undergo the type-I spinning motion. In Section 3.1, we introduce a set of model equations. We additionally introduced an antisymmetric tensor variable, which is directly related to an angular momentum, to the coupled equations of motion of the velocity of the centre of mass and the symmetric deformation tensor representing a deformable self-propelled particle, which is discussed in Section 2.3 of the previous chapter. The numerical simulation of the model equations as well as the theoretical analysis is developed in

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Section 3.2. Finally we summarise and conclude this chapter with Section 3.3.¹

As we will see in the next Chapter 4, the model for the type-I spinning motion is not applicable for the type-II spinning motion since the type-II spinning motion is not necessarily related to the rotation of the whole body and hence, to the angular momentum [113]. Indeed, the active rotation, i.e., the spontaneous rotation of the whole particle, is not necessary for a deformable particle to exhibit the type-II spinning motion.

3.1 Spinning motion with active rotation

Besides the translation of the centre of mass, the rotation around the centre of mass is another relevant degree of freedom. This fact implies the possible existence of active rotation. That is, the active particle may undergo a rotational motion around its centre of mass spontaneously. The spinning motion due to this active rotation is referred to as a type-I spinning motion in this thesis, which is what we are interested in this chapter. Since the type-I spinning motion is the resulting motion of the active rotation, it is related to the spinning motion of a rigid body, for which an angular momentum and hence an angular velocity can be defined. In this section, we first introduce time-evolution equations where the couplings among the migration, rotation, and deformation of the active particle are taken into consideration. By solving the equations of motion numerically, the dynamics of active deformable particles that undergo the spinning motion of type I are studied in detail in the following section. Some of the bifurcations are also obtained analytically.

3.1.1 Time-evolution equations

Our analysis in this thesis is based on the equations of motion derived from symmetry arguments. Here we take into consideration the velocity of the center of mass $\mathbf{v}$, a traceless symmetric tensor variable $\mathbf{S}$ representing an elliptical deformation, and an antisymmetric tensor variable $\mathbf{\Omega}$ characterising the rotation of the particle. The resulting coupled equations of motion are²³

$$\frac{dx_i}{dt} = v_i \tag{3.1}$$

$$\frac{dv_i}{dt} + a_0^r \Omega_{ik} v_k = -\kappa_1 v_i - a_0 (v_k v_k) v_i - a_1 S_{ik} v_k \tag{3.2}$$

¹ This chapter is a review of the publications by the author of this thesis [77, 111, 112]. The numerical simulation in the chapter is newly carried out for this thesis.

² If the antisymmetric tensor variable $\mathbf{\Omega}$ is not considered, the set of equations (3.1)–(3.3) reduces to the set of equations of motion (2.29)–(2.31), which has been described in Section 2.3.1.

³ The term with the coefficient b_1^r in Eq. (3.3) has been corrected [127]. In Ref. [111], it was $\Omega_{ik} S_{k\ell} \Omega_{\ell j}$. Its trace $\Omega_{mk} S_{k\ell} \Omega_{\ell m}$ vanishes in two dimensions, while in a three-dimensional space generally remains finite. Therefore, this correction of the term with b_1^r does not change the results in a two-dimensional space at all, which is the case we consider in this thesis.

3.1 Spinning motion with active rotation

$$\begin{aligned} \frac{dS_{ij}}{dt} + b_0^r (\Omega_{ik}S_{kj} + \Omega_{jk}S_{ki}) \\ = -\kappa_2 S_{ij} - b_0 (S_{kl}S_{kl}) S_{ij} + b_1 \left(v_i v_j - \frac{v_k v_k}{d} \delta_{ij} \right) \\ + b_1^r \left(\Omega_{ik}S_{kl}\Omega_{lj} - \frac{\Omega_{mk}S_{kl}\Omega_{lm}}{d} \delta_{ij} \right) + b_2^r (\Omega_{kl}\Omega_{kl}) S_{ij} \end{aligned} \quad (3.3)$$

$$\frac{d\Omega_{ij}}{dt} = \zeta \Omega_{ij} - o_0 (\Omega_{kl}\Omega_{kl}) \Omega_{ij} + o_1 (\Omega_{ik}S_{kj} - \Omega_{jk}S_{ki}) + o_2 S_{ik}\Omega_{kl}S_{lj} \quad (3.4)$$

where a_1 , a_0^r , b_1 , b_0^r , b_1^r , b_2^r , o_1 and o_2 are coupling constants. d is the spatial dimension. The parameters κ_1 and ζ characterise the internal forces for active propulsion and for active rotation respectively, and κ_2 represents the relaxation rate of the deformation. Here, we consider the case with positive κ_2 , such that the shape of the particle becomes circular when there is no coupling between the shape deformation and the active velocity or the active rotation.

The meaning of each coupling term in Eqs. (3.2)–(3.3) is as follows. The third term on the right-hand side of Eq. (3.2) and the second term on the right-hand side of Eq. (3.3) are the couplings of the velocity and the deformation to the leading order, where the migration induces the deformation (b_1 term) and the deformation reduces the velocity (a_1 term). The coupling term with a_1 also has an effect to bend the migration direction depending on the parameters. The second term on the left-hand side of Eq. (3.2) with $a_0^r > 0$ corresponds to the force known as a Magnus effect, where a particle suffers a force in the direction perpendicular to that of the translational velocity and the angular velocity. As a result, the trajectory of a rotating particle tends to be curved. The second term on the left-hand side of Eq. (3.3) with $b_0^r > 0$ represents the rotation of the configuration around $\boldsymbol{\omega}$.⁴ The third and fourth terms on the right-hand side of Eq. (3.3) coincide in a two-dimensional space but a factor 2, i.e. $2b_1^r \Omega_{ik}S_{kl}\Omega_{lj} = b_2^r (\Omega_{kl}\Omega_{kl}) \Omega_{ij}$, both of which have the same tendency⁵ to enhance the elliptical deformation due to the rotation for b_1^r , $b_2^r > 0$. The terms with the coefficient o_1 and o_2 on the right-hand side

⁴ The same procedure is applicable for higher mode deformations. For example, the rotation of the triangular deformation due to the rotation Ω is included via $\Omega_{im}U_{mjk} + \Omega_{jm}U_{mki} + \Omega_{km}U_{mij}$. Therefore, the equation of motion for the third-order deformation tensor $\mathbf{U}$ becomes

$$\frac{dU_{ijk}}{dt} + c_0^r (\Omega_{im}U_{mjk} + \Omega_{jm}U_{mki} + \Omega_{km}U_{mij}) = -\kappa_3 U_{ijk} - c_0 (U_{lmn}U_{lmn}) U_{ijk} + (\text{coupling terms}). \quad (3.5)$$

In the same way, the time-evolution equation of the fourth-order deformation tensor $\mathbf{T}$ becomes

$$\begin{aligned} \frac{dT_{ijkl}}{dt} + e_0^r (\Omega_{im}T_{mjkl} + \Omega_{jm}T_{mkli} + \Omega_{km}T_{mlji} + \Omega_{lm}T_{mijk}) \\ = -\kappa_4 T_{ijkl} - e_0 (T_{i'j'k'\ell'} T_{i'j'k'\ell'}) T_{ijkl} + (\text{coupling terms}). \end{aligned} \quad (3.6)$$

⁵ Although the term with $b_2^r > 0$ reduces the stiffness of the elliptical deformation and hence enhances the deformation uniformly, in a three-dimensional space the term with b_1^r enhances the deformation in the direction perpendicular to $\boldsymbol{\omega}$ for $b_1^r > 0$. Besides, it has an additional meaning to rotate the configuration around an axis perpendicular to $\boldsymbol{\omega}$.

If b_1^r , $b_2^r < 0$, the opposite effect takes place; That is, the active rotation reduces the elliptical deformation.

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of Eq. (3.4) have the same effect on the vector ω but from the deformation parallel and perpendicular to it respectively. Both of them weaken the rotation for deformed particle if $o_1, o_2 > 0$. Therefore, the second term on the right-hand side of Eq. (3.4) with the coefficient o_1 vanishes in a two-dimensional space.

In Ref. [111], we have investigated the spinning dynamics in two dimensions obtained from Eqs. (3.2)–(3.4) by varying κ_1 and b_2^r with a fixed positive value of ζ . In this situation, the dynamics of a deformable self-propelled particle with a finite active rotational force ζ have been considered. The coefficient κ_1 governs the migration velocity and is a fundamental parameter. Our concern was the effect of the coupling of the active rotation and the deformations on the particle dynamics. Therefore, we varied the coefficients b_2^r .

On the other hand, in Ref. [112], we have investigated the dynamics near the bifurcation where the active rotation Ω appears. In other words, we were interested in how the active deformable particle achieves the active rotation. In the following, we describe the dynamics in this situation. To this end, all the coefficients, $a_1, a_0^r, b_1, b_0^r, b_1^r, b_2^r, o_1$, and o_2 , are fixed, while the parameters κ_1 and ζ are varied. The deformability of the particle κ_2 is also fixed.

3.2 Dynamics of active deformable particle with active rotation

In this section, we investigate the emergence of the active rotation. Due to the couplings among the active translational and rotational motions and the shape deformation of the particle, the dynamics around the region where the active rotation Ω appears, i.e. $\zeta \approx 0$, are not trivial. We first show the results of the numerical simulations and then develop analytical investigations of some of the bifurcations.

3.2.1 Numerical simulations

In order to solve Eqs. (3.1)–(3.4) numerically in two dimensions, we employ the fourth-order Runge-Kutta method with the time increment $\Delta t = 10^{-3}$. Since we are interested in the dynamics around the region $\zeta \approx 0$, we vary ζ , representing the strength of the internal rotation, as well as κ_1 , characterising the internal propulsion strength. In numerical simulations, we fix the deformability of the elliptical deformation as $\kappa_2 = 0.5$. Other coefficients are set as $a_0 = 1, a_1 = b_1 = -1, a_0^r = b_0^r = 1, b_1^r + 2b_2^r = 1, o_0 = 0.5$ and $o_2 = 1$.

The results are summarised in Fig. 3.1. In Fig. 3.1(a), we show the dynamical phase diagram. The different symbols indicate the different dynamical states, which we will discuss shortly. In each of the panel sets, Figs. 3.1(b)–(h), the trajectory in real space is plotted in the first column. The time dependence of the angles of the velocity ϕ and the elliptical deformation θ_2 are plotted by the solid and dotted lines in the upper panel of the second column, while that of their magnitudes v and s_2 as well as the value of the active rotation ω are displayed by the solid, dotted, and dashed lines in the lower panel of the second column. The upper and lower panels of the third column show the relation of ω and v as well as that of s_2 and the relative angle $\psi = \theta_2 - \phi$, respectively.

3.2 Dynamics of active deformable particle with active rotation

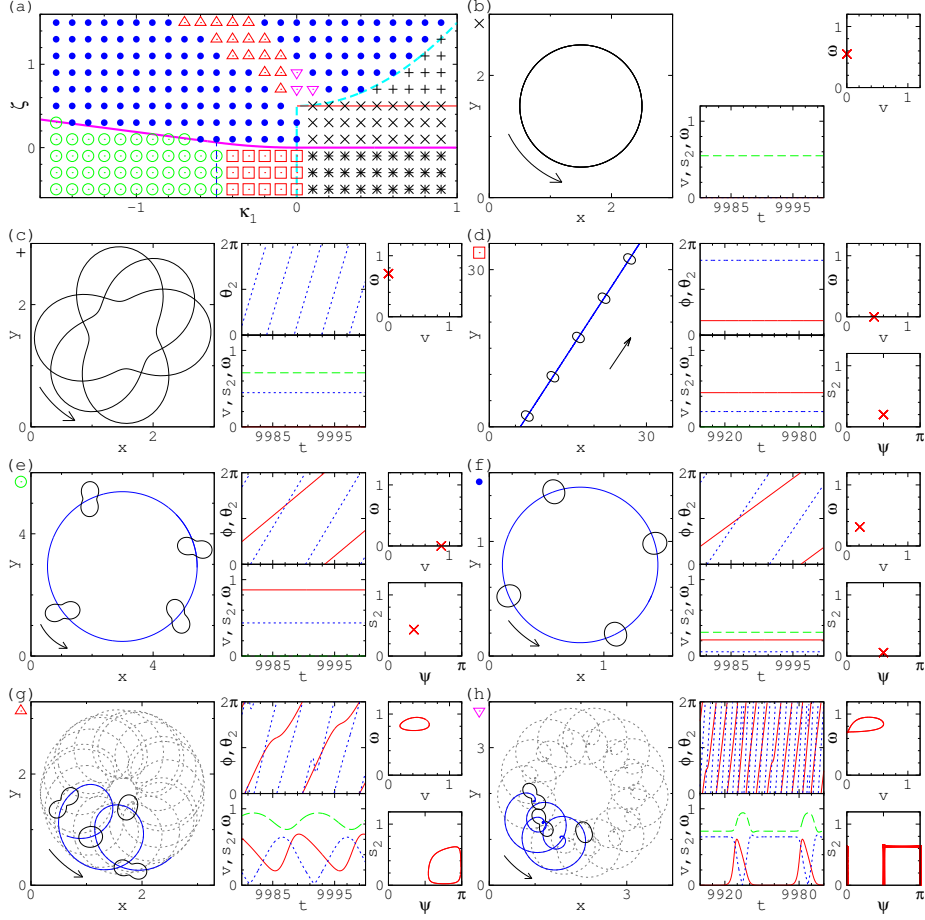


Figure 3.1: (a) Dynamical phase diagram and (b)–(h) typical dynamical states with their trajectory in real space (the first column), the time series of the angles ϕ and θ_2 (the upper panel of the second column), that of v , s_2 , and ω (the lower panel of the second column), and the trajectories in ω - v space (the upper panel of the third column) and in s_2 - ψ space (the lower panel of the third column); (b) *circular-spinning motion* for $\kappa_1 = 0.5$ and $\zeta = 0.3$; (c) *deformed-spinning motion* for $\kappa_1 = 0.5$ and $\zeta = 0.7$; (d) *straight motion* for $\kappa_1 = -0.4$ and $\zeta = -0.1$; (e) *circular motion* for $\kappa_1 = -1$ and $\zeta = -0.1$; (f) *orbital revolution* for $\kappa_1 = -0.1$ and $\zeta = 0.1$; (g) *quasi-periodic motion* for $\kappa_1 = -0.1$ and $\zeta = 0.9$; and (h) *intermittent quasi-periodic motion* for $\kappa_1 = 0$ and $\zeta = 0.9$. In the panel (a), the thin solid and broken lines represent the bifurcation boundaries between the circular-spinning and deformed-spinning states and between the straight and circular states, respectively. The thick broken and thick solid lines are the stability limit of $v = 0$ given by Eq. (3.19) and that of $\omega = 0$ given by Eq. (3.23). In the panes (d)–(h), some particle snapshots are superposed to the trajectory, the size of which is adjusted for illustration. In the panels (g) and (h), trajectories for long-time intervals are plotted by black dotted lines with short-time trajectories emphasised by the blue solid lines. The gray arrows in the panels (b)–(h) indicate the directions of motion. In the panes (b), (c) and (e)–(h), particles undergoes the counter-clockwise rotation. These are obtained by solving Eqs. (3.1)–(3.4) numerically.

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The stars in Fig. 3.1(a) represent the parameter region where the motionless circular-shaped particle without deformation is found. The regions indicated by the cross and plus symbols in Fig. 3.1(a) correspond to the spinning motions without and with the elliptical deformation, where the centre-of-mass position is motionless. The latter is referred to as a *deformed-spinning state* to distinguish from the former, which is named a *circular-spinning state* in this chapter. The circular-spinning state and the deformed-spinning state are depicted in Fig. 3.1(b) for $\kappa_1 = 0.5$ and $\zeta = 0.3$ and in Fig. 3.1(c) for $\kappa_1 = 0.5$ and $\zeta = 0.7$, respectively. From these figures, it is obvious that there exists finite active rotation $\omega \neq 0$ for both of the circular-spinning motion and the deformed-spinning motion. This concludes that these two spinning motions are the type-I spinning motion. Since the particle at the circular-spinning motion does not exhibit any deformation and has a circular shape, it is hard to see that it is really rotating unless a marker point is put onto it. Still the value of ω takes a finite value, indicating that it undergoes a spinning motion. The angles ϕ and θ_2 are not defined, and so is their relative angle ψ , since the velocity and the elliptical deformation do not exist for the circular-spinning motion, and thus the plot of them are not available in Fig. 3.1(b). Similarly, the angles ϕ and ψ is not defined for the deformed-spinning motion, the plot related to these values does not appear in Fig. 3.1(c).

The open square symbol in Fig. 3.1 represents a *straight state*, where a particle propels in a straight line with its shape elliptically deformed and without active rotation $\omega = 0$. In the region indicated by the open circle, an elliptically-deformed particle undergoes an orbital revolution in a circular trajectory without active rotation $\omega = 0$. This orbital revolution is due to the coupling of the spontaneous propulsion and the deformability of the particle. We call this state as a *circular state*. Figures 3.1(d) and (e) display examples of the straight state for $\kappa_1 = -0.4$ and $\zeta = -0.1$ and the circular state for $\kappa_1 = -1$ and $\zeta = -0.1$, respectively. For the trajectory in real space, some snapshots of the particle are superposed, the size of which is adjusted for illustration. To draw the snapshots of the particle, the radius is set to 1 throughout this chapter.

There also exist orbital revolutions with finite active rotation $\omega \neq 0$. The filled circles in Fig. 3.1(a) represent the region where a particle undergoes an orbital revolution due to finite active rotation with its shape elliptically-deformed⁶. The sign of ω takes both plus and minus depending on the initial condition. We call this an *orbital revolution* in this chapter, which is depicted in Fig. 3.1(f) for $\kappa_1 = -0.1$ and $\zeta = 0.1$.

Particles in the region of the top and down triangles in Fig. 3.1(a) undergo quasi-periodic motions, with their shape elliptically-deformed and with a finite active rotation. In the latter case (the top triangles), the particle moves in an intermittent manner as shown in Fig. 3.1(f) for $\kappa_1 = 0$ and $\zeta = 0.9$. Therefore, we call this an *intermittent-quasi-periodic motion* to distinguish from the former one, which is simply referred to

⁶ In our previous papers [111, 112], we found two types of orbital revolution with finite active rotation with different directions of the deformation with respect to the velocity, given by the variable $\psi = \theta_2 - \phi$. In those cases, we have chosen different values for a_0^r and b_0^r ($a_0^r = 0.75$ and $b_0^r = 1$). However, we here consider the same value for them, i.e. $a_0^r = b_0^r = 1$, which we think is the reason why only one type of orbital revolution with finite active rotation exists.

a *quasi-periodic motion*, in this thesis.⁷ The trajectories of the quasi-periodic motion and the intermittent-quasi-periodic motion are depicted in Fig. 3.1(g) for $\kappa_1 = -0.1$ and $\zeta = 0.9$ and in Fig. 3.1(h) for $\kappa_1 = 0$ and $\zeta = 0.9$. The value of ω is positive in Figs. 3.1(g) and (h), where the particle moves counter-clockwise direction. However, the sign of ω takes both plus and minus depending on the initial condition.

Finally, we briefly mention bifurcation lines in Fig. 3.1(a). The thick solid line indicates the stability limit of $\omega = 0$, below which $\omega = 0$ is stable whereas it takes a finite value otherwise. The thick dashed line represents the stability limit of $v = 0$, on the right of which v vanishes and on the left side of which v takes a finite value. The thin solid line is the bifurcation threshold between the circular-spinning motion the elliptical spinning motion, while the thin dashed line denotes the bifurcation line between the straight motion and the circular motion. These lines are obtained analytically, the formulae of which and its derivation will be discussed in the following.

3.2.2 Theoretical analysis

We now develop theoretical analysis of the bifurcation around where the particle achieves the active velocity and the active rotation, respectively. To this aim, we consider the stabilities of the solutions with $v = 0$ and of those with $\omega = 0$, one by one. We describe the velocity $\mathbf{v}$, the elliptical deformation $\mathbf{S}$, and the active rotation Ω with the magnitudes and the characteristic angles:

$$v_1 = v \cos \phi, \quad v_2 = v \sin \phi, \quad (3.7)$$

$$S_{11} = -S_{22} = s_2 \cos 2\theta_2, \quad S_{12} = S_{21} = s_2 \sin 2\theta_2, \quad (3.8)$$

$$\Omega_{11} = \Omega_{22} = 0, \quad \Omega_{12} = -\Omega_{21} = \omega. \quad (3.9)$$

Then, Eqs. (3.2)–(3.4) become

$$\frac{dv}{dt} = -\kappa_1 v - a_0 v^3 - a_1 v s_2 \cos 2\psi, \quad (3.10)$$

$$\frac{d\phi}{dt} = -a_1 s_2 \sin 2\psi + a_0^r \omega, \quad (3.11)$$

$$\frac{ds_2}{dt} = -\kappa_2 s_2 - 2b_0 s_2^3 + \frac{b_1}{2} v^2 \cos 2\psi + (b_1^r + 2b_2^r) s_2 \omega^2, \quad (3.12)$$

$$\frac{d\theta_2}{dt} = -\frac{b_1 v^2}{4s_2} \sin 2\psi + b_0^r \omega, \quad (3.13)$$

$$\frac{d\omega}{dt} = -\zeta \omega - 2o_0 \omega^3 - o_2 s_2^2 \omega, \quad (3.14)$$

⁷ In our pervious works [111, 112], we have distinguished two types of quasi-periodic motion, where on the one hand the relative angle ψ oscillates with in a finite values between 0 and π just as our current quasi-periodic motion but on the other hand ψ varies from 0 to π . We do not find the latter quasi-periodic motion in our current case, the reason of which we think is again the choice of the same value for a_0^r and b_0^r .

Furthermore, we have found a chaotic behaviour via period doubling for large ζ in our previous paper [111], which is also not found in our current simulation.

We did not aware of the intermittent-quasi-periodic motion previously.

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where we have written $\psi = \theta_2 - \phi$. Since the dynamics (3.10)–(3.14) are determined by v , s_2 , ω , and ψ , equations that we have to solve is Eqs. (3.10), (3.12), and (3.14) as well as

$$\frac{d\psi}{dt} = \left(a_1 s_2 - \frac{b_1 v^2}{4s_2} \right) \sin 2\psi + (-a_0^r + b_0^r) \omega. \quad (3.15)$$

When the particle does not exhibit active rotation, i.e., $\omega = 0$, the solutions of Eqs. (3.10), (3.12), and (3.15) are the same as those obtained in Section 2.3.1 of the previous chapter. There are three types of solutions. One is a trivial one, i.e., $v = 0$ and $s_2 = 0$, which corresponds to a motionless circular-shaped particle without deformation. In this case, the angle ϕ and θ_2 lose their meaning, so does their relative angle ψ . This solution is stable as long as $\kappa_1 > 0$. For $\kappa_1 < 0$, the solutions of Eqs. (3.10) and (3.12) is calculated as

$$v = \left(\frac{-2\kappa_1 \kappa_2}{2\kappa_2 a_0 + a_1 b_1 \cos 2\psi} \right)^{1/2} \quad \text{and} \quad s_2 = \frac{-\kappa_1 b_1 \cos 2\psi}{2\kappa_2 a_0 + a_1 b_1 \cos^2 2\psi}. \quad (3.16)$$

There are two possible solutions of Eq. (3.15) for Eq. (3.16). One is given by $\tan 2\psi = 0$ and the other by

$$\cos^2 2\psi = \frac{2a_0 \kappa_2^2}{a_1 b_1 (-2\kappa_1 - \kappa_2)}. \quad (3.17)$$

The set of solution, Eq. (3.16) and $\tan 2\psi = 0$, represents a straight motion where the particle undergoes a migration in a straight line, while the set of solutions, Eqs. (3.16) and (3.17), indicates a circular motion where the centre of mass of the particle draws a circular trajectory. The former is stable as long as $\kappa_1^c < \kappa_1 < 0$ whereas the stability condition of the latter is given by $\kappa_1 < \kappa_1^c$. Here the bifurcation boundary between the straight and circular motions are calculated as

$$\kappa_1^c = -\frac{a_0}{a_1 b_1} \kappa_2^2 - \frac{1}{2} \kappa_2. \quad (3.18)$$

For these solutions, the stability of $\omega = 0$ is given from Eq. (3.14) by $Z < 0$, where

$$Z \equiv \zeta - o_2 s_2^2 = \begin{cases} \zeta & \text{for the motionless state} \quad \text{i.e. } \kappa_1 > 0 \\ \zeta - o_2 \left(\frac{-\kappa_1 b_1}{2a_0 \kappa_2 + a_1 b_1} \right)^2 & \text{for the straight state} \quad \text{i.e. } \kappa_1^c < \kappa_1 < 0 \\ \zeta - o_2 \frac{b_1 (-2\kappa_1 - \kappa_2)}{8a_0 a_1} & \text{for the circular state} \quad \text{i.e. } \kappa_1 < \kappa_1^c \end{cases} \quad (3.19)$$

When the particle does not exhibit a translational motion, there are again three solutions of Eqs. (3.12)–(3.14). One is a trivial solution same as the one above, i.e., $v = s_2 = \omega = 0$, for which the relative angle ψ loses its meaning. The trivial solution is

stable as long as $\kappa_1 > 0$ and $\zeta < 0$ (See also Eq. (3.19)). The other solutions are given by

$$s_2 = 0 \quad \text{and} \quad \omega = \pm \left(\frac{\zeta}{2o_0} \right)^{1/2}, \quad (3.20)$$

and

$$s_2 = \left(\frac{-2o_0\kappa_2 + \zeta(b_1^r + 2b_2^r)}{o_2(b_1^r + 2b_2^r)} \right)^{1/2} \quad \text{and} \quad \omega = \pm \left(\frac{\kappa_2}{b_1^r + 2b_2^r} \right)^{1/2}. \quad (3.21)$$

The former set of solutions, Eq. (3.20), represents a spinning circular particle without deformation, which is stable as long as $0 < \zeta < \zeta^*$. The latter, Eq. (3.21), corresponding to a spinning elliptically-deformed particle, the stability of which is given by $\zeta > \zeta^*$. Here, we have defined

$$\zeta^* = \frac{2\kappa_2 o_0}{b_1^r + 2b_2^r}. \quad (3.22)$$

For these solutions, the stability condition of $v = 0$ is calculated from Eq. (3.10) as $G < 0$, where

$$\begin{aligned} G &\equiv -\kappa_1 - o_0 s_2 \cos 2\psi \\ &= \begin{cases} -\kappa_1 & \text{for } \zeta < \zeta^* \\ -\kappa_1 + |a_1| \left(\frac{-2o_0\kappa_2 + \zeta(b_1^r + 2b_2^r)}{o_2(b_1^r + 2b_2^r)} \right)^{1/2} & \text{for } \zeta > \zeta^* \end{cases} \end{aligned} \quad (3.23)$$

The resulting bifurcation lines are superposed to the phase diagram in Fig. 3.1(a). The line of the stability limit for $\omega = 0$, given by $Z = 0$ with Z defined by Eq. (3.19), is plotted by the thick solid line in Fig. 3.1(a). The stability threshold of the motionless centre-of-mass position, i.e. $v = 0$, which is obtained as $G = 0$ with G given by Eq. (3.23), is displayed by the thick dashed line in Fig. 3.1(a). Furthermore, the bifurcation threshold between the straight motion and the circular motion, given by $\kappa_1 = \kappa_1^c$ with Eq. (3.18), and the bifurcation line between the circular-spinning motion and the deformed-spinning motion, given by $\zeta = \zeta^*$ with ζ^* defined by Eq. (3.22), are drawn by the thin dashed line and the thin solid line in Fig. 3.1(a), respectively. As shown in Fig. 3.1(a), these analytical thresholds are consistent with the results of the numeral simulations.

3.3 Summary and conclusions

In summary, we address that there exist at least two types of spinning motion regarding an active deformable particle. One is a spinning motion (type-I spinning motion) due to the rotation of the whole body, which corresponds to the spinning motion of a rigid body. The other spinning motion (type-II spinning motion) is related to traveling waves of deformation along the interface.

In this chapter, we considered a model of the former spinning motion (type-I). We studied the dynamics of a deformable self-propelled particle with spontaneous rotation, where two different types of activeness were taken into account. One is active propulsion,

3 Two types of spinning motion

where the center of mass of the particle spontaneously undergoes a translational motion due to its internal driving force. The other is active rotation, where the configuration of the particle rotates spontaneously around its center of mass. In our previous paper [111], we investigated the dynamics of a deformable self-propelled particle with finite active rotation in a two-dimensional space. Contrary, in this chapter, we were concerned with the dynamics around the emergence of the active rotation [77, 112].

We first introduced equations of motion for active deformable particle from symmetry considerations for the particle centre-of-mass position $\mathbf{x}$ and its velocity $\mathbf{v}$, the elliptical deformation $\mathbf{S}$, and the active rotation Ω . We have solved the time-evolution equations (3.1)–(3.4) numerically, and obtained a rich variety of dynamical states as summarised in a dynamical phase diagram for $\kappa = 0.5$ displayed in Fig. 3.1. Apart from the motionless, straight, and circular states, where the active rotation vanishes, we have found an orbital revolution state, quasi-periodic state, and an intermittent-quasi-periodic state as well as spinning motions with and without deformation, both of which are of type I, when finite active rotation exists.

In addition to the numerical simulations, the emergence of the active rotation ω have been investigated analytically by the stability analysis of the active rotation for the motionless, straight, and circular states, where the active rotation does not exist $\omega = 0$. The stability of $v = 0$ has also been analysed theoretically for the motionless state, the circular-spinning state, and the deformed-spinning state. The results are superposed to the phase diagram in Fig. 3.1(a), which show good agreement with the results of the numerical simulations.

To conclude, we clarified that the type-I spinning motion can be described by using an antisymmetric tensor of second order, which is related to the angular velocity of the particle. By using this expression, we can include the (active) rotation of the particle in the same sense as the symmetric deformation tensors. Moreover, the equations of motion for these variables as well as the centre-of-mass velocity were systematically derived from symmetry arguments.

Future problems should be addressed from a theoretical viewpoint. The derivation of the equations of motion (3.1)–(3.4) from continuous models is an open problem. A difficulty already lays when to derive the rotation of the particle from a continuous model. The next step is how to include different time scales for the rotation and the deformations as well as the centre-of-mass velocity.

In the next section, we will investigate the type-II spinning motion and will see how it is different from the type-I spinning motion discussed in this chapter.

Chapter 4

Spinning motion without active rotation

Spinning motion is a relevant basic spontaneous movement of active matter. Indeed, both synthetic and biological active matters are found to exhibit a spinning motion [8, 40, 49, 116–121, 123, 124]. In particular, for a deformable particle, there are at least two types of spinning motion. One is due to the rotation of the whole body, which is called a type-I spinning motion in this thesis. As discussed in the previous chapter, for the type-I spinning motion, an angular momentum can be defined in the same way as for a classical rigid body [125, 126].

Contrary, a deformable particle can undergo a spinning motion even without rotating the whole body. If the shape of the particle is deformable and does change in time, the deformation may travel along the interface of the particle. This traveling wave of deformation along the interface results in a spinning motion in terms of the dynamics of the particle, which we call a type-II spinning motion in this thesis. In this case, the interfacial motion plays an important role and the whole body of the particle does not necessarily rotate.

Such a spinning motion is indeed obtained in experiments. Recently, the dynamical relations of the shape deformation and the centre-of-mass movement of living organisms are experimentally analysed [49, 124], where the spinning motion appears due to the traveling wave of deformation. Furthermore, the internal chemical reaction of living cell that induces deformation of the cell membrane has also visualised [8], where a spiral wave of chemical reaction was observed.

In this chapter we introduce and study a theoretical model of active deformable particles that reproduce the type-II spinning motion. In Section 4.1, we consider an active deformable particle in a quiescent environment and develop a set of model equations by taking into account limited modes of deformation. We then emphasise a special symmetry of the coupled equations for different deformation modes in Section 4.2. The emergence of the type-II spinning motion is discussed analytically in Section 4.3 and the prediction is verified numerically in Section 4.4. Finally, Section 4.5 is devoted to the summary and conclusions of this chapter. The relation of the centre-of-mass velocity and shape deformations are briefly discussed in Appendix 4.A. The argument developed in this chapter is one of the main issues of this thesis, and it is based on the author's

previous study published in Ref. [113].¹

4.1 Time-evolution equations

In order to emphasise that the type-II spinning motion does occur independent of the rotation of the whole body, we do not consider the active rotation Ω in this chapter. Instead we here take into account the shape deformations, as well as the velocity of the centre of mass $\mathbf{v}$, up to the fourth modes: $\mathbf{S}$, $\mathbf{U}$, $\mathbf{T}$. We derive the time-evolution equations for these variables based on the consideration of the two fundamental symmetries, i.e. the uniformity and isotropy of space. The set of equations is constructed such that the translational symmetry and the rotational symmetry are satisfied. The couplings of the velocity and the deformations are considered up to the quadratic nonlinearity. The resulting time-evolution equations are

$$\frac{dx_i}{dt} = v_i, \quad (4.1)$$

$$\frac{dv_i}{dt} = -\kappa_1 v_i - a_0 (v_m v_m) v_i + a_1 S_{im} v_m + a_2 U_{imn} S_{mn} + a_3 T_{imnp} U_{mnp}, \quad (4.2)$$

$$\begin{aligned} \frac{dS_{ij}}{dt} = & -\kappa_2 S_{ij} - b_0 (S_{mn} S_{mn}) S_{ij} \\ & + b_1 \left[v_i v_j - \frac{v_m v_m}{2} \delta_{ij} \right] + b_2 U_{ijm} v_m + b_3 T_{ijmn} S_{mn}, \end{aligned} \quad (4.3)$$

$$\begin{aligned} \frac{dU_{ijk}}{dt} = & -\kappa_3 U_{ijk} - c_0 (U_{mnp} U_{mnp}) U_{ijk} \\ & + c_1 \left[v_i S_{jk} + v_j S_{ki} + v_k S_{ij} - \frac{v_m}{2} (\delta_{ij} S_{km} + \delta_{jk} S_{im} + \delta_{ki} S_{jm}) \right] + c_2 T_{ijkm} v_m, \end{aligned} \quad (4.4)$$

$$\begin{aligned} \frac{dT_{ijkl}}{dt} = & -\kappa_4 T_{ijkl} - e_0 (T_{mnpq} T_{mnpq}) T_{ijkl} \\ & + e_1 \left[S_{ij} S_{kl} + S_{ik} S_{jl} + S_{il} S_{jk} - \frac{S_{mn} S_{mn}}{4} (\delta_{ij} \delta_{kl} + \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) \right] \\ & + e_2 \left[U_{ijk} v_l + U_{lij} v_k + U_{kli} v_j + U_{jkl} v_i \right. \\ & \left. - \frac{v_m}{3} (\delta_{ij} U_{klm} + \delta_{ik} U_{jlm} + \delta_{il} U_{kjm} + \delta_{jk} U_{ilm} + \delta_{jl} U_{ikm} + \delta_{kl} U_{ijm}) \right]. \end{aligned} \quad (4.5)$$

Here κ_1 is a friction coefficient of the centre of mass, whereas κ_2 , κ_3 , and κ_4 represent stiffness of the second-, third-, and fourth-mode deformations, respectively. If these

¹ The content of this chapter is basically the same as those in the publication by the author of this thesis in Ref. [113]. However, although the time-evolution equations in Ref. [113] are described in terms of Fourier components, we employ the tensor description of the variables in this thesis. Therefore, the results of numerical simulation in this chapter, as well as the figure 4.1, are newly produced for this thesis. This modification is only for the description of the formulae and does not change the physics itself.

coefficients may take positive values, the cubic terms with positive coefficients a_0 , b_0 , c_0 , and e_0 are required to avoid divergence. The other coefficients are phenomenological parameters of the couplings among the velocity and the deformations.

In what follows, we take account of only the second- and fourth-order deformations. The situation is justified if the friction κ_1 is so large that the centre of mass of the particle hardly translate, i.e. $\mathbf{v} = \mathbf{0}$. Then, from Eq. (4.4), the third-order symmetric tensor $\mathbf{U}$ is determined independent of the other two variables, i.e. $\mathbf{S}$ and $\mathbf{T}$. Furthermore, from Eqs. (4.3) and (4.5), the contribution of the third-order tensor on the dynamics of the second- and fourth-order tensors vanishes if $\mathbf{v} = \mathbf{0}$. Therefore, we only have to consider the coupled equations of the second- and the fourth-order deformations, Eqs. (4.3) and (4.5), as long as the centre of mass of the particle is motionless. In the followings, we therefore investigate the coupled equations of motion for the second- and fourth-mode deformations, Eqs. (4.3) and (4.5).

4.2 Special symmetry

Before investigating the coupled dynamics of the second- and the fourth-mode deformations, we here emphasise that there is a special symmetry among the equations of motion. From Eqs. (4.2)–(4.5), the first and second modes constitute a set of coupled equations:

$$\frac{dv_i}{dt} = -\kappa_1 v_i - a_0 (v_m v_m) v_i + a_1 S_{im} v_m, \quad (4.6)$$

$$\frac{dS_{ij}}{dt} = -\kappa_2 S_{ij} - b_0 (S_{mn} S_{mn}) S_{ij} + b_1 \left[v_i v_j - \frac{v_m v_m}{2} \delta_{ij} \right]. \quad (4.7)$$

For the sake of clarity, we have ignored the third- and fourth-order deformations by putting $\mathbf{U} = \mathbf{0} = \mathbf{T}$ in Eqs. (4.2)–(4.3) to obtain the above set of equations. In a similar way, a set of coupled equations of second- and fourth-order deformations must take the following form:

$$\frac{dS_{ij}}{dt} = -\kappa_2 S_{ij} - b_0 (S_{mn} S_{mn}) S_{ij} + b_3 T_{ijmn} S_{mn}, \quad (4.8)$$

$$\begin{aligned} \frac{dT_{ijkl}}{dt} = & -\kappa_4 T_{ijkl} - e_0 (T_{mnpq} T_{mnpq}) T_{ijkl} \\ & + e_1 \left[S_{ij} S_{kl} + S_{ik} S_{jl} + S_{il} S_{jk} - \frac{S_{mn} S_{mn}}{4} (\delta_{ij} \delta_{kl} + \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) \right]. \end{aligned} \quad (4.9)$$

Mathematically, Eqs. (4.8) and (4.9) have the same structures as Eqs. (4.6) and (4.7). This is a consequence of the possible couplings of the n th- and $2n$ th-order deformations, and hence, it is independent of any details of the system considered.²

²To see this fact, it is more convenient to write down the equations by using Fourier components:

$$\frac{dz_n}{dt} = -\kappa_n z_n - \mathcal{A}_0 (z_n z_{-n}) z_n + \mathcal{A}_1 z_{2n} z_{-n}, \quad (4.10)$$

$$\frac{dz_{2n}}{dt} = -\kappa_{2n} z_{2n} - \mathcal{B}_0 (z_{2n} z_{-2n}) z_{2n} + \mathcal{B}_1 z_n z_n. \quad (4.11)$$

The above fact implies that bifurcation structures that Eqs. (4.6) and (4.7) exhibit should also occur for the coupled equations (4.8) and (4.9). As we have seen in Section 2.3.1, it is known that, in the dynamics governed by Eqs. (4.6) and (4.7), a bifurcation between a straight motion and a circular motion appears for $-\kappa_1 > 0$ and $\kappa_2 > 0$ [110]. Then a question arises; What kinds of dynamics appear in Eqs. (4.8) and (4.9) as a corresponding bifurcation, which we shall address below.

4.3 Emergence of time-dependent deformations and spinning motion

In this and the next sections, we consider the dynamics when both of the second- and fourth-order deformations, $\mathbf{S}$ and $\mathbf{T}$, may occur spontaneously. This is the case where both κ_2 and κ_4 can take negative values in Eqs. (4.8) and (4.9). In this situation, the terms with positive values of b_0 and e_0 should be kept in Eqs. (4.8) and (4.9) to avoid a divergence. It is noted here that if the coefficients b_3 and e_1 have the same sign, Eqs. (4.3) and (4.5) are variational, which is not the case we are interested in in this thesis. Therefore, we concentrate on the case $b_3 e_1 < 0$. We first develop an analytical investigation of the solutions and their stabilities of the coupled equations (4.8) and (4.9) in this section, and show the results of the numerical simulation in the next section.

In order to solve Eqs. (4.8) and (4.9) analytically, we rewrite the symmetric tensors $\mathbf{S}$ and $\mathbf{T}$ with the magnitudes and directions by using the relation given in Eqs. (2.12) and (2.18): $S_{11} = -S_{22} = s_2 \cos 2\theta_2$ and $S_{12} = s_2 \sin 2\theta_2$, and $T_{1111} = T_{2222} = -T_{1122} = s_4 \cos 4\theta_4$ and $T_{1112} = -T_{1222} = s_4 \sin 4\theta_4$. The time-evolution equations (4.8) and (4.9) then become

$$\frac{ds_2}{dt} = -\kappa_2 s_2 - 2b_0 s_2^3 + 2b_3 s_2 s_4 \cos \Theta_{24}, \quad (4.12)$$

$$2s_2 \frac{d\theta_2}{dt} = 2b_3 s_2 s_4 \sin \Theta_{24}, \quad (4.13)$$

$$\frac{ds_4}{dt} = -\kappa_4 s_4 - 8e_0 s_4^3 + \frac{3}{2} e_1 s_2^2 \cos \Theta_{24}, \quad (4.14)$$

$$4s_4 \frac{d\theta_4}{dt} = -\frac{3}{2} e_1 s_2^2 \sin \Theta_{24}, \quad (4.15)$$

where $\Theta_{24} \equiv 4\theta_4 - 4\theta_2$. From Eqs. (4.12)–(4.15), the dynamics is determined by s_2 , s_4 and Θ_{24} . Therefore, the time-evolution equations we need to consider is Eqs. (4.12) and (4.14) as well as

$$\frac{d\Theta_{24}}{dt} = -\Lambda(s_2, s_4) \sin \Theta_{24}, \quad (4.16)$$

where we have written

$$\Lambda(s_2, s_4) = \frac{3e_1}{2s_4} s_2^2 + 4b_3 s_4. \quad (4.17)$$

First, we investigate the stationary solutions of Eqs. (4.12), (4.14), and (4.16), as well as their stability. The stationary solutions of Eq. (4.16) is immediately obtained:

In principle, this set of equations can be formulated with deformations described in tensor forms.

4.3 Emergence of time-dependent deformations and spinning motion

$\sin \Theta_{24} = 0$ and by $\Lambda(s_2, s_4) = 0$, where s_2 and s_4 are respectively given from Eqs. (4.12) and (4.14) as functions of Θ_{24} . As usual, the stability of the stationary solutions is analysed by using the linear stability matrix [128] defined by

$$\mathcal{L}_{ij} = \frac{\partial}{\partial \mathcal{X}_j} \frac{d\mathcal{X}_i}{dt}, \quad (4.18)$$

where $\mathcal{X}_i \in \{s_2, s_4, \Theta_{24}\}$. In a special case, that is, for the stationary solution of Eq. (4.16) given by $\sin \Theta_{24} = 0$, the stability of Eq. (4.16) and that of Eqs. (4.12) and (4.14) are decoupled, and hence, can be considered separately. The linear stability matrix of Eqs. (4.12) and (4.14) is defined by

$$L_{ij} = \frac{\partial}{\partial s_j} \left(\frac{ds_i}{dt} \right), \quad (4.19)$$

and the stability of the solution $\sin \Theta_{24} = 0$ is given by

$$L_{\Theta_{24}} = -\Lambda \cos \Theta_{24} < 0. \quad (4.20)$$

When $L_{\Theta_{24}} > 0$, the stationary solution of Θ_{24} is obtained from $\Lambda = 0$.

Equations (4.12) and (4.14) have a pair of trivial solutions, $s_2 = s_4 = 0$, which represents a motionless circular-shaped particle without deformations. The stability of this solution is given, from Eq. (4.19), by

$$\kappa_2 > 0 \quad \text{and} \quad \kappa_4 > 0. \quad (4.21)$$

Since the magnitudes of the second and fourth-mode deformations are zero, their angles θ_2 and θ_4 lose their meaning, and therefore, it is unnecessary to consider Eq. (4.16) and its stability Eq. (4.20).

For the trivial solution $s_2 = 0$ of Eq. (4.12), there is another solution of Eq. (4.14), which is calculated as $s_4^2 = -\kappa_4/8e_0$, where $\kappa_4 < 0$ is required since $e_0 > 0$. From the stability matrix (4.19), one can obtain the stability condition of the pair of solutions $s_2 = 0$ and $s_4 = \sqrt{-\kappa_4/8e_0}$ as

$$\kappa_4 < 0 \quad \text{and} \quad \kappa_2 > b_3 \sqrt{\frac{-\kappa_4}{2e_0}} \cos 4\Theta_{24}. \quad (4.22)$$

This gives the stability condition of a motionless particle with static fourth-mode deformation. Here, note that, although the angle θ_2 is not defined for $s_2 = 0$, we may consider it around the bifurcation where s_2 becomes finite, and hence, $\Theta_{24} = 4\theta_4 - 4\theta_2$ is given from Eq. (4.16) with $\sin \Theta_{24} = 0$.

Now, the non-trivial stationary solution of Eq. (4.12) is obtained as

$$s_2 = \left\{ \frac{-\kappa_2 + 2b_3 s_4 \cos \Theta_{24}}{2b_0} \right\}^{1/2}. \quad (4.23)$$

For this solution, the solution s_4 of Eq. (4.14) satisfies

$$16b_0 e_0 s_4^3 + (2b_0 \kappa_4 - 3b_3 e_1 \cos^2 \Theta_{24}) s_4 + \frac{3}{2} \kappa_2 e_1 \cos \Theta_{24} = 0. \quad (4.24)$$

4 Spinning motion without active rotation

Since Eq. (4.24) is cubic with respect to s_4 , the solution can be solved analytically, but we do not write down the explicit form here.

When the solution of Eq. (4.16) is given by $\sin \Theta_{24} = 0$, the angles θ_2 and θ_4 are both time independent as is obvious from Eqs. (4.12) and (4.14). Therefore, the set of solutions given by of Eqs. (4.23) and (4.24) represents a motionless particle with static second- and fourth-mode deformations. The stability condition of this state is obtained from Eqs. (4.19) and (4.20). As a result of a straightforward calculation of the stability analysis, it is found that there are at least three possibilities of bifurcations. Two of them are obtained from the 2×2 matrix L given by Eq. (4.19) [128]. One is given by the condition that the determinant of the stability matrix becomes zero, $\det L = 0$, where one of the eigenvalues changes its sign from negative to positive. The other is a Hopf bifurcation given by the trace of the stability matrix, i.e. $\text{tr } L = 0$. As long as Eq. (4.20) is satisfied, it is expected from Eqs. (4.13) and (4.15) that the magnitudes of the second- and fourth-mode deformations undergo oscillations beyond this Hopf bifurcation threshold keeping their direction $2\theta_2$ and $4\theta_4$ time independent. The third possible bifurcation is given by $L_{\Theta_{24}} = 0$, where the stationary solution of the angles $\sin 4\Theta_{24} = 0$ becomes unstable. In this case, from Eqs. (4.13) and (4.15), the angles θ_2 and θ_4 become time dependent and vary in time. As a result, a spinning motion may occur above the instability threshold. Since the active rotation is absent here, this spinning motion is definitely different from the type-I spinning motion in the previous chapter. Indeed, since the deformation of the particle shape that travels along the interface is crucial, this spinning motion is what we refer to as a type-II spinning motion in this thesis.

When the stationary solution Θ is given by $\Lambda = 0$, the solution s_4 of Eq. (4.24) with Eq. (4.23) represents a spinning motion, where a particle with second- and fourth-mode deformations rotates around its motionless centre of mass. The analytical form of this solution is obtained from Eqs. (4.17), (4.23), and (4.24) as

$$s_2^2 = \frac{-b_3(2\kappa_2 + \kappa_4)}{4b_0b_3 - 3e_0e_1}, \quad (4.25)$$

$$s_4^2 = \frac{3e_1(2\kappa_2 + \kappa_4)}{8(4b_0b_3 - 3e_0e_1)}, \quad (4.26)$$

$$\cos \Theta_{24} = -\frac{3\kappa_2e_0e_1 + 2\kappa_4b_0b_3}{3b_3e_1(2\kappa_2 + \kappa_4)} \left\{ \frac{6e_1(2\kappa_2 + \kappa_4)}{4b_0b_3 - 3e_0e_1} \right\}^{1/2}. \quad (4.27)$$

The stability condition of the spinning motion is obtained from the real part of the eigenvalues of the stability matrix $\mathcal{L}$ given by Eq. (4.18). The characteristic equation of $\mathcal{L}$ is written as $\lambda^3 - I_{\mathcal{L}}\lambda^2 + II_{\mathcal{L}}\lambda - III_{\mathcal{L}} = 0$, where $I_{\mathcal{L}}$, $II_{\mathcal{L}}$, and $III_{\mathcal{L}}$ are the first, second, and third invariants of the stability matrix $\mathcal{L}$. Here, we note that the first and third invariants are nothing but the trace and the determinant, respectively, whereas the second invariant is defined by

$$II_{\mathcal{L}} = \frac{1}{2} \left\{ (\text{tr } \mathcal{L})^2 - \text{tr } \mathcal{L}^2 \right\}. \quad (4.28)$$

To proceed the calculation, it is convenient to introduce

$$\mathcal{P} = -\frac{1}{9}I_{\mathcal{L}}^2 + \frac{1}{3}II_{\mathcal{L}}, \quad (4.29)$$

$$\mathcal{Q} = -\frac{1}{27}I_{\mathcal{L}}^3 + \frac{1}{6}I_{\mathcal{L}}II_{\mathcal{L}} - \frac{1}{2}III_{\mathcal{L}}, \quad (4.30)$$

with which the characteristic equation can be written by $\lambda'^3 + 3\mathcal{P}\lambda' + 2\mathcal{Q} = 0$, where we have written $\lambda' = \lambda - I_{\mathcal{L}}/3$. From a straightforward calculation, we obtain the stability limit of the spinning motion as follows. First, if $\mathcal{Q}^2 + \mathcal{P}^3 > 0$, the spinning state becomes unstable by a pitchfork bifurcation or by a Hopf bifurcation. The pitchfork bifurcation boundary is given by

$$\mathcal{U}_+ + \mathcal{U}_- + \frac{1}{3}I_{\mathcal{L}} = 0, \quad (4.31)$$

whereas the Hopf bifurcation boundary is obtained as

$$-\frac{1}{2}(\mathcal{U}_+ + \mathcal{U}_-) + \frac{1}{3}I_{\mathcal{L}} = 0. \quad (4.32)$$

Here we have defined

$$\mathcal{U}_+ = \left[-\mathcal{Q} + (\mathcal{Q}^2 + \mathcal{P}^3)^{1/2} \right]^{1/3}, \quad (4.33)$$

$$\mathcal{U}_- = \left[-\mathcal{Q} - (\mathcal{Q}^2 + \mathcal{P}^3)^{1/2} \right]^{1/3}. \quad (4.34)$$

Note that both $\mathcal{U}_{\pm}$ are real for $\mathcal{Q}^2 + \mathcal{P}^3 > 0$. On the other hand, if $\mathcal{Q}^2 + \mathcal{P}^3 < 0$, the spinning motion loses its stability by a pitchfork bifurcation, the threshold of which is obtained as

$$2(-\mathcal{P})^{1/2} \cos \left(\frac{1}{3} \arccos \left(-\mathcal{Q}(-\mathcal{P})^{-3/2} \right) \right) + \frac{1}{3}I_{\mathcal{L}} = 0. \quad (4.35)$$

To summarise, the spinning motion loses its stability by a Hopf bifurcation or by a pitchfork bifurcation. After the Hopf bifurcations, an oscillation of the magnitude of deformations for the spinning particle is expected to occur.

4.4 Numerical results

In this section, we show the results of numerical simulations of Eqs. (4.8) and (4.9) and compare them with the analytical results obtained in the preceding section. In order to solve Eqs. (4.8) and (4.9) numerically, we have varied the parameters κ_2 and κ_4 whereas the coupling constants fixed as $b_0 = 1 = e_0$, $b_3 = -\sqrt{2}$ and $e_1 = \sqrt{2}/3$. The fourth-order Runge-Kutta method has been employed with the time increment $\delta t = 10^{-3}$.

The results are summarised in Fig. 4.1, where the dynamical phase diagram is displayed in Fig. 4.1(a) with the bifurcation lines obtained in Section 4.3 and in Figs. 4.1(b)–(i) particle silhouettes of each dynamical states are depicted. Different symbols in Fig. 4.1(a) represent different solutions. The stars in Fig. 4.1(a) indicate the region

4 Spinning motion without active rotation

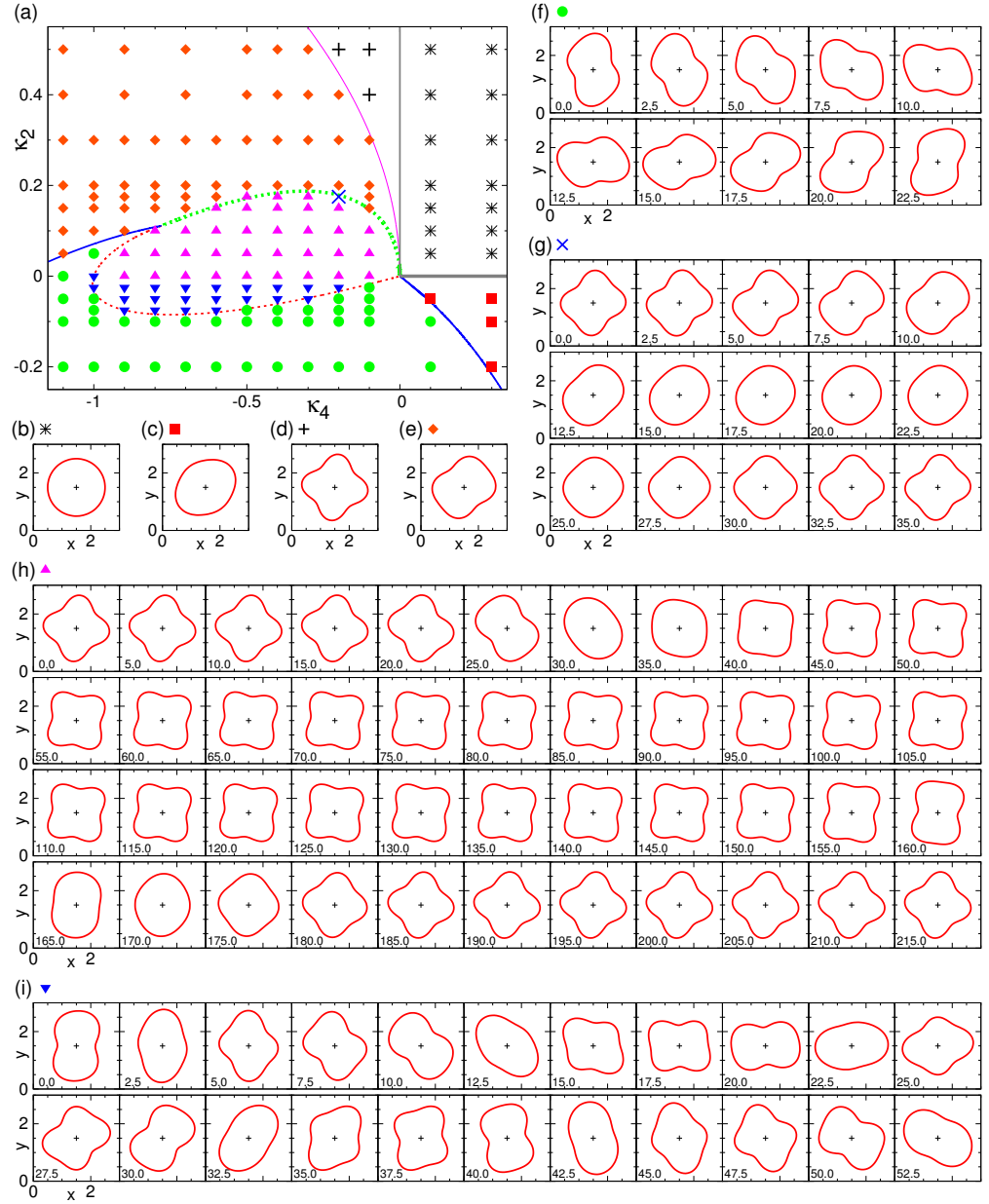


Figure 4.1: (a) Dynamical phase diagram and (b)–(i) silhouettes of the particle at each dynamical states. The symbols at the panels (b)–(i) correspond to those in the phase diagram in the panel (a). The small pluses in the panel (b)–(i) indicate the centre-of-mass position of the particle. Time series of the *type-II spinning motion*, *oscillation*, *intermittent-oscillation*, and *oscillatory-spinning* motions are respectively displayed in the panels (f)–(i) with the time interval $\Delta t = 2.5$. These are obtained by solving Eqs. (4.8) and (4.9) numerically for $b_0 = 1 = e_0$, $b_3 = -\sqrt{2}$ and $e_1 = \sqrt{2}/3$. The bifurcation lines obtained analytically in Section 4.3 are superposed in the panel (a).

where particles are motionless with undeformed circular shape as shown in Fig. 4.1(b) for $\kappa_2 = 0.1$ and $\kappa_4 = 0.3$, whereas the plus symbol in Fig. 4.1(a) stands for the parameters of the motionless particles with only a static fourth-order deformation as depicted in Fig. 4.1(d) for $\kappa_2 = 0.5$ and $\kappa_4 = -0.2$. Motionless particles with static second- and fourth-order deformations are found in the region denoted by the square and diamond symbols as respectively displayed in Fig. 4.1(c) for $\kappa_2 = -0.1$ and $\kappa_4 = 0.3$ and in Fig. 4.1(e) for $\kappa_2 = 0.2$ and $\kappa_4 = -0.2$, where the relative directions of the second- and fourth-order deformations are different.

In the region indicated by the circle, a particle with both second- and fourth-order static deformations rotates around its centre of mass. For this motion, the shape of the particle is time independent when observed from the co-rotating frame. Since the active rotation Ω is absent in Eqs. (4.8) and (4.9), this spinning motion actually is the *type-II spinning motion*. The time series of the type-II spinning state is displayed in Fig. 4.1(f) for $\kappa_2 = -0.05$ and $\kappa_4 = -0.2$ with the time interval $\Delta t = 2.5$. Besides the type-II spinning motion, a particle with second- and fourth-order deformations can experience an oscillation of the deformations at the region indicated by the cross symbols in Fig. 4.1(a). A time series of this *oscillation state* of the deformations are displayed in Fig. 4.1(g) for $\kappa_2 = 0.175$ and $\kappa_4 = -0.2$ with the times interval $\Delta t = 2.5$. In the region represented by the up triangles, the particle with the second- and fourth-order deformations undergoes a standing oscillation as shown in Fig. 4.1(h) for $\kappa_2 = 0.15$ and $\kappa_4 = -0.2$ with the time interval $\Delta t = 2.5$. Note that, compared to the oscillation state in Fig. 4.1(g), this oscillatory motion is intermittent, and hence, referred to as an *intermittent oscillation* in this chapter. In the region indicated by the down-triangle symbols, the *oscillatory-spinning motion* appears, where the particle with the second- and fourth-order deformations undergoes both a standing oscillation and a spinning motion. The time series of this state is depicted in Fig. 4.1(i) for $\kappa_2 = -0.025$ and $\kappa_4 = -0.2$ with time interval $\Delta t = 2.5$.

Finally, we briefly mention the bifurcation boundaries of different dynamical states in the phase diagram. The lines in Fig. 4.1(a) are the bifurcation thresholds obtained analytically in Section 4.3. The gray thick and thin solid lines are the stability limits of the motionless circular particle without deformation given by Eq. (4.21), whereas the magenta solid line is the bifurcation line between the motionless particle only with a static fourth-order deformation and the motionless particle with static second- and fourth-order deformations, obtained from Eq. (4.22). The blue thin solid lines are the bifurcation threshold between the motionless deformed state with static second- and fourth-order deformations and the spinning motion, given by Eq. (4.31). Here, note that we have checked numerically that this line coincides with the pitchfork bifurcation line obtained from $L_\Theta = 0$ with $\text{tr } L < 0$ and $\det L > 0$ for the set of solutions (s_2, s_4, Θ_{24}) given by Eqs. (4.23) and (4.24) together with $\sin \Theta_{24} = 0$. For this set of solutions, there is another bifurcation line displayed by the green thin dotted line in Fig. 4.1(a). This is the Hopf bifurcation line of the motionless deformed state with static second- and fourth-order deformations, given by $\text{tr } L = 0$ with $L_\Theta < 0$ and $\det L > 0$. Beyond this Hopf bifurcation, an oscillatory motion appears as predicted in Section 4.3. The red dotted line is the Hopf bifurcation boundary of the type-II spinning motion, which

is obtained from Eq. (4.32).

As mentioned in section 4.2, the coupled equations for the second- and fourth-mode deformations have the same structure as those for the first-mode deformation, which actually is the centre-of-mass velocity, and the second-mode deformation. In fact, we note that the motionless state with static second- and fourth-mode deformations, the type-II spinning motion, the intermittent oscillation, and the oscillatory-spinning motion respectively correspond to the straight motion, the circular motion, the rectangular motion, and the quasiperiodic motion, which are obtained in the dynamics of the first- and the second-order Fourier modes [109, 113]. The oscillation state corresponds to the oscillatory straight motion discussed in Section 2.3 of Chapter 2, both of which have been overlooked in previous studies [109, 113]. The corresponding bifurcation lines have been obtained for the equations of motion of the centre-of-mass velocity and the elliptical deformation in Ref. [109] except for the Hopf bifurcation line indicated by the red dotted line [113].

4.5 Summary and conclusions

To summarise this chapter, we have investigated the type-II spinning motion as the dynamics of an active deformable particle, which experiences spontaneous shape deformation. The time-evolution equations for the deformation tensors are constructed up to the fourth-order deformations and the couplings of different modes are considered up to the second orders for simplicity.

We have first clarified the existence of a special symmetry between the coupled equations of n th- and $2n$ th-mode deformations for different integers n . As an example, we have compared the dynamics obtained for the coupled time-evolution equations of the first- and second-mode deformations, and for the equations of the second- and fourth-mode deformations.

In order to clarify the existence of the type-II spinning motion, we investigated a set of coupled equations of motion for the second- and fourth-order deformations. From the stability analysis of the steady solutions, we predicted the existence of the spinning motion and the oscillation of deformations, as well as the motionless particle with static deformations, for the equations of second- and fourth-mode deformations. For these dynamical states, time-dependent deformations play important roles. Furthermore, we do not take into consideration the antisymmetric tensor Ω , characterising the rotation of the whole particle. Thus, the spinning motion obtained in this chapter is definitely the type-II spinning motion. The analytical formulae of the bifurcations were also obtained.

We also solved the time-evolution equations numerically. The results are summarised in Fig. 4.1. All the predicted dynamical states as well as the intermittent oscillation of deformations and the oscillatory-spinning motion, where the oscillation of the deformation occurs in addition to the spinning motion, are numerically reproduced. Moreover, all the bifurcations of different solutions, except the bifurcation between the oscillation state and the intermittent oscillation state and the bifurcation between the intermittent oscillation state and the oscillatory-spinning state, are obtained analytically, and

moreover, consist with the numerical results as in Fig. 4.1.

In Section 2.3.1 of Chapter 2, we have introduced the dynamics of the coupled equations of motion for the first- and second-mode deformations [109, 110]. As we have discussed in Chapter 2, the first-mode deformation results in the displacement of the centre of mass, and hence, can be included in the velocity of the centre of mass. Therefore, despite the mathematical equivalence of the time-evolution equations, the actual dynamics we have obtained in this chapter for the time-evolution equations of the second- and fourth-mode deformations represents physically different behavior from those obtained in Section 2.3.1 and Refs. [109, 110].

We make a remark about ignoring of the third mode in the present investigation. The results obtained for the second- and fourth-mode deformations are justified as long as we are considering the situation that the center of mass of the particle is motionless. In that case, we may put, as shown in Appendix 4.A, all the modes with odd integers identically equal to zero.

In conclusion, in the previous and present chapters, we have clarified our claim that there are, at least, two different types of spontaneous spinning motions of a deformable particle. One is the case where a particle undergoes a spinning motion due to the rotation of the whole body, as discussed in the previous chapter. This type-I spinning motion has been modelled by introducing the antisymmetric tensor representing angular velocity as a dynamic variable, which couples with the migration velocity and the deformation tensors [111, 112, 129]. On the other hand, the type-II spinning motion is related to the excitation of a propagating wave on the surface of a deformable particle as described in the present chapter. Then, a question arises as to how one can distinguish experimentally these two different kinds of spinning motions. We do not have any conclusive answer for this at the moment. However, one of the possibilities is to look for standing oscillation by changing the system parameters since such an oscillation never emerges in the type-I spinning motion caused by the angular momentum. In fact, in Ref. [49], both a spontaneous spinning motion and a standing oscillation have been observed.

Finally, we briefly mention the dimensionality of space. In this chapter, we have considered a spontaneous spinning motion only in two dimensions. In fact, most of the experiments of living cells such as protozoa are carried out on a substrate and hence, regarded as quasi-two-dimensional. However, there are many biological objects [51] and nonbiological droplets [34, 130] that undergo a three-dimensional self-propelled motion. Therefore, it is interesting to extend the present theory to three dimensions. However, a rotational motion in three dimensions is not necessarily axial symmetric. It has been shown that a helical motion appears already for coupled equations of the centre-of-mass velocity and the second-order deformation in addition to a circular motion [131]. Therefore the structure of bifurcations is expected to be more complex compared to two dimensions and systematic studies are needed. We shall return to this problem somewhere in the near future.

4.A Velocity of the centre of mass

The velocity of the center of mass can be written as [105]

$$\mathbf{v} = \frac{1}{\Omega} \int d\omega V(\omega) \mathbf{R}(\omega), \quad (4.36)$$

where Ω is the area of the particle and

$$d\omega = R\sqrt{1 + (R'/R)^2}d\phi, \quad V = \frac{dR/dt}{\sqrt{1 + (R'/R)^2}}, \quad (4.37)$$

with $R' = \partial R/\partial\phi$. The position vector $\mathbf{R}$ is given by a complex representation as $\mathbf{R} = R(\phi)e^{i\phi}$. Since $R(\phi)$ is given by Eq. (2.6) with (2.7) excluding $m = \pm 1$ modes, the integrand $d\omega V \mathbf{R}$ must take a factor $d\phi e^{im\phi+i\phi}$ with m even integer when δR contains only the modes with even integers—in other words, the case that $m = -1$ is totally excluded. Therefore, after integral over $0 < \phi < 2\pi$, the velocity of the center of mass $\mathbf{v}$ vanishes identically.

Chapter 5

Dynamics of active deformable particle under shear flow

In a quiescent environment, dynamical equations of motion of active deformable particles were recently put forward where the couplings between the particle propulsion and its deformability are taken into consideration [12, 53–55, 109–113, 131, 132], some of which have been introduced in the previous chapters. One of the unexpected results was a spontaneous circling motion due to the coupling of the deformability and the self-propulsion [109, 110, 131]. However, in most practical situations [84, 133, 134], various external fields are present to influence the particle motion. They are induced by, for instance, chemoattractant, phototaxis, and gravity [135–139], or external walls [117, 118, 140, 141]. An important particular case is a solvent flow field such as a Couette flow with a constant shear gradient or a Poiseuille flow through tubes. There are several studies of rigid self-propelled particles in various shear geometries [142–145]. However, despite its practical relevance, the motion of a deformable self-propelled particle in a solvent flow had not been considered theoretically before our study [114]. The corresponding modelling is expected to be complex since already rigid (undeformable) active particles have been shown to perform periodic motion on cycloids (rather than on straight lines) once they are exposed to a linear shear flow field [144].

In this chapter we close this gap and propose a theoretical model for the motion of an active deformable particle in an external flow field. We use symmetry considerations to obtain coupled nonlinear dynamical equations for the particle position, velocity, deformation, and its active rotation. In our model, the passive rotation induced by the external flow and the active rotation are both taken into account. By using the obtained equations, we theoretically explore the motion of a deformable active particle in a linear shear flow in the latter half of this chapter and in a swirl in the next chapter.

In particular, we clarify the fact that our equations reduce to known models in the two limits of vanishing shear flow and vanishing particle deformability. On the one hand, for vanishing shear flow, our equations reduce to previous models for deformable particles [77, 110–112]. On the other hand, for vanishing particle deformability, we obtain the cycloidal motion as embodied in previous investigations [144]. For varied shear rate and particle propulsion speed, we solve the equations numerically and obtain a manifold

of different dynamical modes including active straight motion, periodic motions, regular and undulated cycloidal motions, winding motions, as well as quasi-periodic and chaotic motions induced at high shear rates. The types of motion are distinguished by different characteristics in the dynamical behavior of the particle positions, velocity orientations, and its deformations.

The organisation of this chapter is as follows. We first introduce time-evolution equations for an active deformable particle under an external flow in Section 5.1. In Section 5.2, we consider the special case of a round disk-shaped non-deformable active particle by eliminating the variable for deformation. We relate this case to the previous work [144]. Next, in Section 5.3, we present numerical results for the dynamics of a deformable self-propelled particle without active rotation under a steady shear flow. In Section 5.4, a spontaneous particle rotation for the dynamics is additionally included and the results of the numerical simulations are presented. Finally, Section 5.5 is devoted to the summary and to conclusions of this chapter.

This chapter is one of the main issues of this thesis and is based on the previous study of the present author, which is published in Ref. [114].¹

5.1 Equations of motion of active deformable particle in external flow field

Based on symmetry considerations, we now derive a set of coupled nonlinear dynamical equations to describe the motion of a deformable active particle under an externally imposed flow field. These equations are first listed for the general case of three spatial dimensions and an unspecified flow field. Afterwards we will confine ourselves to a two-dimensional geometry and consider a simple shear flow in the latter half of this chapter. As a first approach, we only investigate the influence of the external flow on the particle dynamics and do not take into account the *inverse* effect.

In the following, we denote the prescribed externally imposed flow field that the particle is exposed to as $\mathbf{u}$. It is a given function of space. To proceed as normal [146, 147], the elongational part and the rotational part of the fluid flow are extracted by the symmetric second-order tensor $\mathbf{A}$ and the antisymmetric second-order tensor $\mathbf{W}$, the components of which are defined in Eq. (2.1) and Eq. (2.2), respectively. We again describe the definition of their components:

$$A_{ij} = \frac{1}{2} (\partial_i u_j + \partial_j u_i), \quad (5.1)$$

$$W_{ij} = \frac{1}{2} (\partial_i u_j - \partial_j u_i). \quad (5.2)$$

As is discussed in Chapter 2, the center-of-mass position of the particle is on the one hand “passively” advected by the externally flow field $\mathbf{u}$ and on the other hand can “actively” self-propel with respect to the surrounding fluid. The corresponding

¹ The content of this chapter is the same as the publication of the author of this thesis in Ref. [114]. The figures, Figs. 5.1, 5.2, and 5.3, are newly produced for this thesis.

5.1 Equations of motion of active deformable particle in external flow field

“active” velocity measured relatively to the surrounding fluid flow is denoted as $\mathbf{v}$. In the same manner, the particle is “passively” rotated by the surrounding flow field as well as can undergo an “active”-spinning motion spontaneously. The rotational contribution of the flow is represented by the antisymmetric tensor $\mathbf{W}$ as mentioned above, where as the active rotation is characterised by the antisymmetric tensor $\mathbf{\Omega}$ as introduced by Eq. (2.4) in Chapter 2. Again we mention that the antisymmetric tensor is related to an angular velocity vector $\boldsymbol{\omega}$ via

$$\Omega_{ij} = \epsilon_{ijk}\omega_k, \quad (5.3)$$

where ϵ_{ijk} denotes the (i, j, k) component of the Levi-Civita tensor. The active rotation $\mathbf{\Omega}$ occurs in addition to the passive rotational motion prescribed by the external flow field $\mathbf{u}$. In other words, the antisymmetric tensor $\mathbf{\Omega}$ measures the relative rotation with respect to the rotational motion $\mathbf{W}$ of the surrounding fluid flow. Therefore, $\mathbf{W} + \mathbf{\Omega}$ describes the total rotation of the particle, or the total angular velocity with respect to the laboratory frame, from which the flow field is parameterized.

Finally, the deformation of the particle can be described by symmetric tensors in a systematic way as discussed in Chapter 2. We here take into consideration only the lowest order deformation, i.e., the second-order deformation $\mathbf{S}$, representing an elliptical deformation (an ellipsoidal deformation in three dimensions) for simplicity.

Altogether, besides the centre-of-mass position $\mathbf{x}$, we have introduced three central dynamical variables to characterise the state of an active deformable particle: a vector $\mathbf{v}$ for the active propulsion velocity, the traceless symmetric tensor of second order $\mathbf{S}$ for the particle deformation, and the antisymmetric tensor $\mathbf{\Omega}$ for the active rotation. Based on symmetry arguments, we derive model equations for the dynamic evolution of these variables, which results in [114]²

$$\frac{dx_i}{dt} = u_i + v_i, \quad (5.4)$$

$$\frac{dv_i}{dt} + a_0^r (W_{ik} + \Omega_{ik}) v_k = -\kappa_1 v_i - a_0(v_k v_k) v_i - a_1 S_{ik} v_k, \quad (5.5)$$

$$\begin{aligned} \frac{dS_{ij}}{dt} + b_0^r [(W_{ik} + \Omega_{ik}) S_{kj} + (W_{jk} + \Omega_{jk}) S_{ki}] \\ = -\kappa_2 S_{ij} + b_1 \left[v_i v_j - \frac{(v_k v_k)}{d} \delta_{ij} \right] \\ + b_1^r \left(\Omega_{ik} S_{kl} \Omega_{lj} - \frac{\Omega_{mk} S_{kl} \Omega_{lm}}{d} \delta_{ij} \right) + b_2^r (\Omega_{kl} \Omega_{kl}) S_{ij} \\ + \nu_1 \left[A_{ij} - \frac{A_{kk}}{d} \delta_{ij} \right] + \nu_2 \left[A_{ik} S_{kj} + A_{jk} S_{ki} - \frac{2}{d} (A_{kl} S_{lk}) \delta_{ij} \right], \end{aligned} \quad (5.6)$$

$$\frac{d\Omega_{ij}}{dt} = \zeta \Omega_{ij} - o_0 (\Omega_{kl} \Omega_{kl}) \Omega_{ij} + o_1 (\Omega_{ik} S_{kj} - \Omega_{jk} S_{ki}) + o_2 S_{ik} \Omega_{kl} S_{lj}. \quad (5.7)$$

² The term with the coefficient b_1^r in Eq. (5.6) has been corrected [148]. In Ref. [114], it was $\Omega_{ik} S_{kl} \Omega_{lj}$, which actually is not traceless in a three-dimensional space, whereas in two dimensions this trace vanishes. Therefore, this correction of the term with b_1^r causes no change of the results in a two-dimensional space at all, which is the case we consider in this thesis.

5 Dynamics of active deformable particle under shear flow

Here δ_{ij} denotes the Kronecker delta, and d is the dimension of space. The coefficients κ_1 , κ_2 , ζ , a_0 , a_1 , b_1 , o_0 , o_1 , o_2 , a_0^r , b_0^r , b_1^r , b_2^r , ν_1 , and ν_2 are phenomenological coupling parameters. In principle, higher-order couplings as well as higher-order deformations can be included, but the present model covers the main physical aspects that we intend to describe.

We comment on each of the terms in this set of time-evolution equations, Eqs. (5.4)–(5.7). First of all, comparing Eqs. (5.4)–(5.7) to Eqs. (3.1)–(3.4) in Chapter 3, one may notice that there is a strong correspondence between them. Indeed, if the flow velocity is switched off, i.e. $\mathbf{u} = \mathbf{0}$ and $\mathbf{A} = \mathbf{W} = \mathbf{0}$, Eqs. (5.4)–(5.7) reduce to Eqs. (3.1)–(3.4). In the presence of the external flow field, the velocity of the particle centre of mass is divided into the surrounding fluid flow velocity $\mathbf{u}$ representing advection and its relative velocity $\mathbf{v}$ due to self-propulsion. Therefore, the time-evolution equation of the center-of-mass position has those two contributions as in Eq. (5.4) for a finite flow velocity, while only the latter contribution enters into Eq. (3.1) where the particle is in a quiescent flow.

In the same way, the rotation of the particle also consists of two contributions, i.e., the “passive” rotation $\mathbf{W}$ and the active rotation $\mathbf{\Omega}$, and thus the total angular velocity of the particle is given by $\mathbf{W} + \mathbf{\Omega}$. In a quiescent flow, the contribution of the active angular velocity $\mathbf{\Omega}$ appears in the terms with the coefficients a_0^r and b_0^r in Eqs. (3.2) and (3.3), which reorient the axes of the active velocity and deformation, respectively. When the particle is placed in a non-vanishing flow field, the active rotation in these terms should be replaced by the total rotation $\mathbf{W} + \mathbf{\Omega}$, as in Eqs. (5.5) and (5.6).³ The terms with b_1^r and b_2^r on the right-hand side of Eq. (5.6), remain same as Eq. (3.3), characterising the internal mechanism where the strength of the deformation changes due to the relative rotation $\mathbf{\Omega}$.⁴ Contrary, the terms with the coefficients ν_1 and ν_2 in Eq. (5.6) represent the elongation of the particle due to the surrounding flow field.⁵ In contrast to Eq. (5.6), the tensor $\mathbf{A}$ containing the elongational part of the fluid flow does not enter Eq. (5.5) for the velocity $\mathbf{v}$. This is because $\mathbf{v}$ is defined as the *relative* velocity with respect to the fluid flow $\mathbf{u}$; See Eq. (5.4). Likewise, the rotational part of the fluid flow characterised by the tensor $\mathbf{W}$ is absent in Eq. (5.7); $\mathbf{\Omega}$ describes the *relative* rotation with respect to the surrounding flow field. In principle, coupling terms between $\mathbf{\Omega}$ and the tensor $\mathbf{A}$ are possible. This would mean that the active particle features a way of reacting to an elongational flow by adjusting its active rotation. However, we do not consider such a process.

The rest of the coupling terms are the same as those in Eqs. (3.2)–(3.4) in chapter 3.

³Since an active particle can follow its own rule to react to the external flow fields, the values of the coefficients a_0^r and b_0^r cannot be generally determined. Here we only assume $a_0^r > 0$ and $b_0^r > 0$, which is related to a Magnus effect, where a force acts onto the particle in the direction perpendicular to its velocity and angular velocity vectors.

⁴When we confine ourselves to a two-dimensional space as we do in the following sections, these two terms are equivalent. We remark that, in a three-dimensional space, the term with the coefficient b_1^r has an additional effect to rotate the particle, unlike the b_2^r term.

⁵These terms are consistent with those of a previous study on the dynamics of a non-active liquid droplet in a fluid flow, where an elliptical shape deformation is taken into account [147, 149].

We note that the contribution with the coefficient ν_2 vanishes for a two-dimensional geometry of incompressible flow. Such a case is studied in this thesis.

The first two terms on the right-hand side of Eq. (5.5) and those of Eq. (5.7) represent the active propulsion for $\kappa_1 < 0$ and the active rotation for $\zeta < 0$, respectively, whereas we assume the second-order deformation relaxes without any coupling with other variables, i.e. $\kappa_2 > 0$. The last term on the right-hand side of Eq. (5.5) and its counterpart, i.e., the second term on the right-hand side of Eq. (5.6) are the leading-order couplings between the active velocity $\mathbf{v}$ and the elliptical deformation $\mathbf{S}$. Due to the latter term with b_1 , the active velocity induces the deformation, and in turn, the deformation reduces the active velocity via the coupling term with a_1 , which also has a tendency to bend the trajectory of the centre of mass for a large active velocity and a large deformation. The last two terms on the right-hand side of Eq. (5.7) have the same effect, to change the active rotational speed depending on the deformation in the perpendicular direction (the term with o_2) and in the parallel direction (the term with o_1) with respect to the angular velocity vector⁶.

Generally our equations apply to a three-dimensional setup. For simplicity, however, we confine ourselves to two spatial dimensions for the remaining part of this chapter and for the next chapter, where we consider two types of external flow field. As the simplest example, we study the case of a linear steady shear flow below. Dynamics of active deformable particles in a swirl, i.e., a vortex flow, are also investigated in the next chapter.

5.2 Dynamics without deformation

For the rest of this chapter, we specify the externally imposed flow field $\mathbf{u}$ to a linear steady shear flow,

$$\mathbf{u} = (\dot{\gamma}y, 0), \quad (5.8)$$

where $\dot{\gamma}$ is the shear rate. We assume $\dot{\gamma}$ is a given constant. The symmetric and antisymmetric parts of its spacial derivative are calculated from Eqs. (5.1) and (5.2) as

$$\mathbf{A} = \begin{bmatrix} 0 & \dot{\gamma}/2 \\ \dot{\gamma}/2 & 0 \end{bmatrix}, \quad (5.9)$$

$$\mathbf{W} = \begin{bmatrix} 0 & -\dot{\gamma}/2 \\ \dot{\gamma}/2 & 0 \end{bmatrix}. \quad (5.10)$$

The full set of dynamic equations (5.4)–(5.7) is very complex. To get a first overview, we start by studying a reduced model. More precisely, we neglect deformability, i.e., we set $\mathbf{S} = 0$, and consider a circularly-shaped rigid particle. Under certain assumptions, an analytical solution can be obtained in this case. Prescribing $\mathbf{S} = 0$, Eq. (5.6) is dropped

⁶ The o_1 term vanishes in two dimensions.

5 Dynamics of active deformable particle under shear flow

from our system of equations. Then, Eqs. (5.4), (5.5), and (5.7) reduce to

$$\frac{dx_i}{dt} = u_i + v_i, \quad (5.11)$$

$$\frac{dv_i}{dt} + a_0^r (W_{ik} + \Omega_{ik}) v_k = -\kappa_1 v_i - a_0 (v_k v_k) v_i, \quad (5.12)$$

$$\frac{d\Omega_{ij}}{dt} = \zeta \Omega_{ij} + o_0 (\Omega_{k\ell} \Omega_{k\ell}) \Omega_{ij}. \quad (5.13)$$

We describe the vector and tensor variables as $\mathbf{x} = (x, y)$,

$$\mathbf{v} = (v \cos \phi, v \sin \phi), \quad (5.14)$$

as well as $\Omega_{11} = \Omega_{22} = 0$ and $\Omega_{12} = -\Omega_{21} = \omega$. Then Eqs. (5.11)–(5.13) become

$$\frac{dx}{dt} = \dot{\gamma} y + v \cos \phi, \quad (5.15)$$

$$\frac{dy}{dt} = v \sin \phi, \quad (5.16)$$

$$\frac{dv}{dt} = -\kappa_1 v - a_0 v^3, \quad (5.17)$$

$$\frac{d\phi}{dt} = a_0^r \left(-\frac{\dot{\gamma}}{2} + \omega \right), \quad (5.18)$$

$$\frac{d\omega}{dt} = \zeta \omega - 2o_0 \omega^3. \quad (5.19)$$

We consider a particle that undergoes both self-propulsion and active rotation, i.e. $\kappa_1 < 0$ and $\zeta > 0$. To solve Eqs. (5.15)–(5.19) analytically, we employ an ansatz that the active velocity v and the active rotation ω relax quickly, and hence, their dynamics can be solved adiabatically by putting $dv/dt = 0$ and $d\omega/dt = 0$ in Eqs. (5.17) and (5.19). Together with $\kappa_1 < 0$ and $\zeta > 0$, we have

$$v = \tilde{v}, \quad (5.20)$$

$$\omega = \tilde{\omega}, \quad (5.21)$$

where

$$\tilde{v} = \left(\frac{|\kappa_1|}{a_0} \right)^{1/2}, \quad (5.22)$$

$$\tilde{\omega} = \pm \left(\frac{\zeta}{2o_0} \right)^{1/2}. \quad (5.23)$$

The positive and negative signs in Eq. (5.23) correspond to the counter-clockwise and clockwise rotation, respectively. With these solutions, Eq. (5.18) reads

$$\frac{d\phi}{dt} = a_0^r \left(-\frac{\dot{\gamma}}{2} + \tilde{\omega} \right). \quad (5.24)$$

From Eqs. (5.15), (5.16), and (5.24) with Eq. (5.20), the trajectory of the center of mass can be calculated as

$$x(t) = \frac{\tilde{v} \{-\dot{\gamma} + a_0^r (-\dot{\gamma}/2 + \tilde{\omega})\}}{\{a_0^r (-\dot{\gamma}/2 + \tilde{\omega})\}^2} \{\sin[\phi(t)] - \sin \phi_0\} + \dot{\gamma} \left\{ \frac{\tilde{v}}{a_0^r (-\dot{\gamma}/2 + \tilde{\omega})} \cos \phi_0 + y_0 \right\} t + x_0, \quad (5.25)$$

$$y(t) = \frac{-\tilde{v}}{a_0^r (-\dot{\gamma}/2 + \tilde{\omega})} \{\cos[\phi(t)] - \cos \phi_0\} + y_0, \quad (5.26)$$

$$\phi(t) = a_0^r \left(-\frac{\dot{\gamma}}{2} + \tilde{\omega} \right) t + \phi_0. \quad (5.27)$$

Here, (x_0, y_0) and ϕ_0 are the position of the center of mass and the direction of the velocity vector at $t = 0$, respectively. This set of solutions draws a cycloidal trajectory.

A similar cycloidal trajectory has previously been obtained for an active rigid particle with a circular shape [144]. In that case, the dynamics of the particle feature a polarity axis [150], the orientation of which in the two-dimensional plane can be characterised by an angle ϕ . It marks the direction of the self-propulsion that generates a relative velocity with respect to the surrounding flow field. The equations of motion introduced in Ref. [144] can be written in the form

$$\frac{dx}{dt} = \dot{\gamma} y + \tilde{\alpha} [\cos \phi + f_x], \quad (5.28)$$

$$\frac{dy}{dt} = \tilde{\alpha} [\sin \phi + f_y], \quad (5.29)$$

$$\frac{d\phi}{dt} = -\frac{\dot{\gamma}}{2} + \tilde{\mu}(1 + g), \quad (5.30)$$

where $\tilde{\alpha}$ is a normalised effective self-propulsion force that is proportional to the self-propulsion velocity $\mathbf{v}$ in the over-damped regime considered in Ref. [144]. $\tilde{\mu}$ accounts for an additional self-induced torque [108] or an externally imposed torque [151] on the particle. Equations (5.28)–(5.30) contain Gaussian white noise terms f_x , f_y , and g , which are not included in the present approach. Our equations (5.15), (5.16), and (5.24), together with the asymptotic steady-state magnitudes of the active velocities in Eqs. (5.20), are consistent with Eqs. (5.28)–(5.30) when the noise terms are neglected. By solving this zero temperature limit for $\tilde{\alpha} = \tilde{v}$ and $\tilde{\mu} = \tilde{\omega}$, one recovers the results presented in Eqs. (5.25)–(5.27) for $a_0^r = 1$.

For the special case of $(\dot{\gamma}/2) = \tilde{\omega}$, the solutions of Eqs. (5.15), (5.16), and (5.24), together with Eq. (5.20), are given by

$$x(t) = \left(\frac{\dot{\gamma}}{2} \tilde{v} \sin \phi_0 \right) t^2 + (\tilde{v} \cos \phi_0 + \dot{\gamma} y_0) t + x_0, \quad (5.31)$$

$$y(t) = (\tilde{v} \sin \phi_0) t + y_0, \quad (5.32)$$

$$\phi(t) = \phi_0. \quad (5.33)$$

The physical meaning of this limit is that the active rotation compensates the passive rotation due to the surrounding flow field, i.e. $\dot{\gamma}/2 = \tilde{\omega}$ in Eq. (5.24) or correspondingly $\dot{\gamma}/2 = \tilde{\mu}$ in Eq. (5.30). Also Eqs. (5.31) and (5.32) are consistent with the ones correspondingly obtained in Ref. [144].

5.3 Dynamics without active rotation

In the previous section, we studied a rigid circular particle without deformation as a first step. We now include deformability, but do not consider the active rotation of the particle. Although various different dynamical states can be found in this situation, the dynamics is still much simpler than that with active rotation, as is shown later. The dynamic equations must be solved numerically.

Choosing $\zeta < 0$ hinders active rotation. To solve Eqs. (5.4)–(5.7), we employ a fourth-order Runge-Kutta method with the time increment $\delta t = 10^{-3}$. We checked the numerical accuracy by comparing results obtained for different time increments.

The full parameter space is far too complex to be exhaustively explored. We therefore concentrate on the impact of only two parameters that we consider central to the current problem. One of them is the strength of the self-propulsion of the particle characterised by the parameter κ_1 . The other one is the strength of the imposed shear flow determined by the shear rate $\dot{\gamma}$.

All coupling parameters are fixed at similar magnitude to allow an equal impact of the corresponding effects on the system behavior. We set $a_0 = 1$, $a_1 = b_1 = -1$, $a_0^r = b_0^r = 1$, $o_0 = 0.5$, $o_1 = \nu_1 = 1$, and $b_1^r + 2b_2^r = 1$ (as noted in Section 5.1 the terms with the coefficients b_1^r and b_2^r coincide in two spatial dimensions, and the terms with the coefficients o_1 and ν_2 vanish in our geometry). Intermediate damping rates are used for the deformations and for the active rotation by imposing $\kappa_2 = 0.5$ and $\zeta = -0.1$, respectively. We obtained our results by directly numerically integrating Eqs. (5.4)–(5.7). After that we reparameterized them for illustrative purposes using Eq. (5.14) and

$$S_{11} = -S_{22} = s_2 \cos 2\theta_2, \quad S_{12} = S_{21} = s_2 \sin 2\theta_2. \quad (5.34)$$

We summarised the results in Fig. 5.1. Figure 5.1(a) shows a dynamical phase diagram in the parameter plane of the self-propulsion strength κ_1 and the shear rate $\dot{\gamma}$. Various qualitatively different types of dynamical states are found and explained in more detail below. They are indicated in the phase diagram by the different symbols. At the position included as $\dot{\gamma} = 0$, we describe in words the type of motion observed at zero shear rate for the different self-propulsion strengths κ_1 . Increasing the shear rate towards the right boundary of the phase diagram, we can see how the shear flow influences the dynamic behavior of the particle.

Each of the observed dynamical states is characterised separately in the rows of Figs. 5.1(b)–(f). The location in the phase diagram is indicated by the corresponding symbol below the panel number. We present typical real-space trajectories by the red dotted lines in the first column. Black arrows indicate the direction of migration. The trajectories are drawn from the laboratory frame. Therefore their appearance strongly

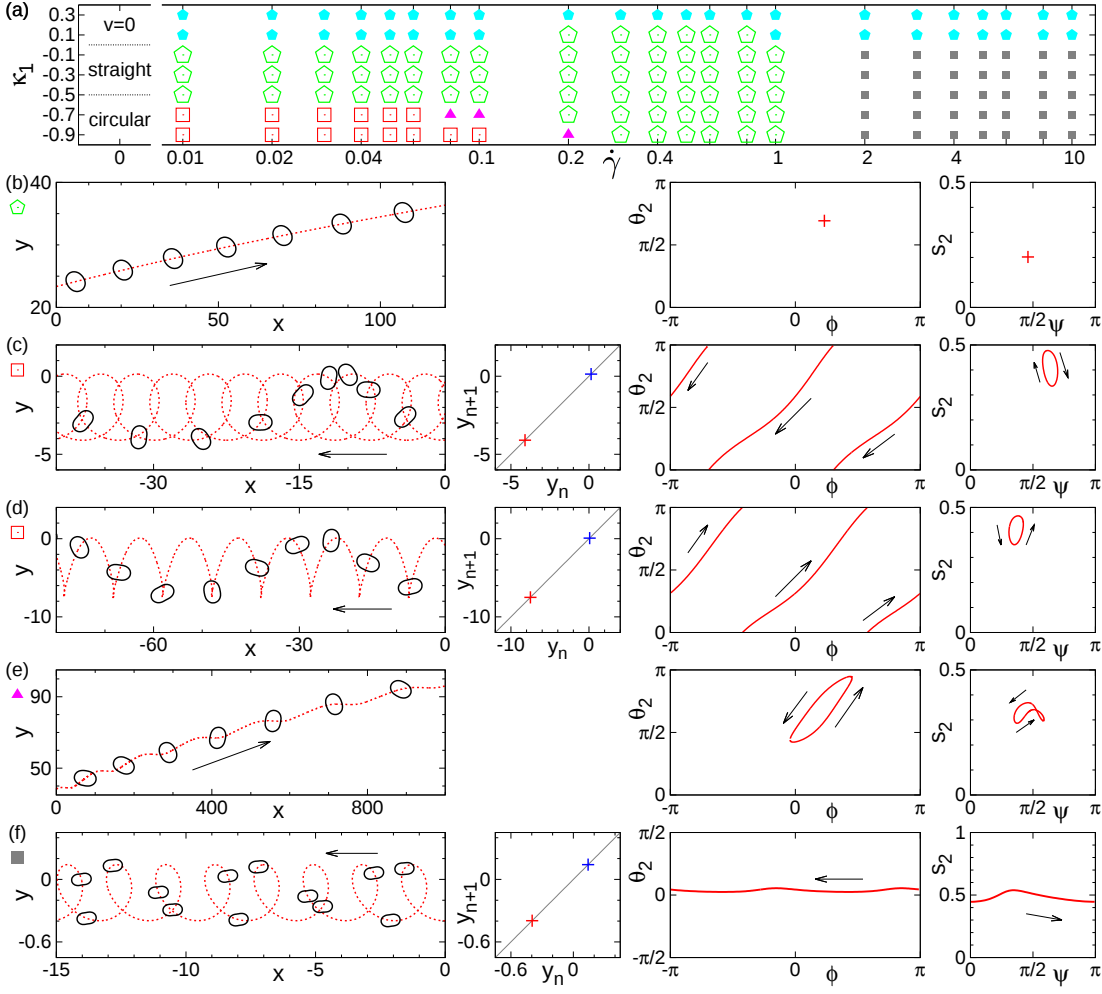


Figure 5.1: (a) Dynamical phase diagram and (b)–(f) trajectories in real space with particle snapshots (1st column), return maps (2nd column), attractors in θ_2 - ϕ space (3rd column) as well as in s - ψ space (4th column) of the typical dynamical motions, obtained by solving Eqs. (5.4)–(5.7) numerically in two dimensions with $\zeta = -0.1$, where the active rotation vanishes $\Omega = 0$. (b) *active straight motion* for $\kappa_1 = -0.5$ and $\dot{\gamma} = 0.1$ indicated by the green open pentagons in panel (a); (c) and (d) *cycloidal I motions* of clockwise and counter-clockwise rotation of the particle deformations, respectively, for $\kappa_1 = -0.9$ and $\dot{\gamma} = 0.1$ marked by the red open squares in panel (a); (e) *winding I motion* for $\kappa_1 = -0.7$ and $\dot{\gamma} = 0.08$ indicated by the purple filled triangles in panel (a); (f) *cycloidal II motion* for $\kappa_1 = -0.1$ and $\dot{\gamma} = 2$ marked by the gray filled squares in panel (a). Arrows in panels (b)–(f) show the directions of motion. Turquoise filled pentagons in panel (a) represent the *passive straight motion* with $v = 0$. Active rotation vanishes $\Omega = 0$ for all of these types of motion. Return map for the *active straight motion* and *winding I motion* in panels (b) and (e) does not exist because the y -component of the velocity does not change its sign in these motions.

depends on the initial y -coordinate: the advective flow velocity increases in y -direction due to the shear geometry and leads to a stretching of the trajectories in x -direction. In particular, the direction of motion also depends on the y -coordinate: the flow field points to the right for $y > 0$, whereas it points to the left for $y < 0$. To avoid confusion, we remark again that the dynamics that is described by Eqs. (5.5)–(5.7) itself is not affected in this way, because only the relative velocity $\mathbf{v}$ with respect to the shear flow velocity is considered and only gradients of the flow velocity enter via the tensors $\mathbf{A}$ and $\mathbf{W}$.

In order to illustrate the current state of deformation and orientation along the trajectories that are drawn in the first column of Figs. 5.1(b)–(f), representative snapshots of the particle are superimposed in black. For the purpose of best visualisation, the size of the particle was adjusted and the deformation does not appear as pure ellipsoids. To further characterise the modes of migration, return maps of the corresponding motion in real space are included in the second column of Figs. 5.1(b)–(f). We extract the local maximum and minimum values of y along each real-space trajectory for several thousand up-down oscillations. The maximum and minimum values are labeled as y_n ($n = 1, 2, \dots$) and plotted as blue and red points, respectively, in the return map y_{n+1} vs. y_n . In other words, we calculated the return maps at the Poincaré sections where $v_y = 0$ for $dv_y/dt < 0$ and $dv_y/dt > 0$, respectively. The diagonal line in the return maps is included for illustration and does not represent any data points.

Finally, the attractors in phase space are drawn in the third and fourth columns. Black arrows indicate the direction of motion along the attractors. We show plots in θ_2 - ϕ space (third column) and in s - ψ space (fourth column). As introduced in Eqs. (5.14) and (5.34), ϕ and θ_2 , which are observed from the laboratory frame, describe the orientation of the relative velocity vector $\mathbf{v}$ and the orientation of the long axis of the deformation tensor $\mathbf{S}$, respectively. This is different for s_2 and ψ . First, s_2 measures the magnitude of deformation as is obvious from the definition of the deformation tensor in Eq. (2.21). Second, ψ is defined as the relative angle between the long axis of deformation and the velocity orientation,

$$\psi = \theta_2 - \phi. \quad (5.35)$$

Thus s_2 and ψ are measured in the co-moving particle frame. Both attractors, in the θ_2 - ϕ space and in the s_2 - ψ space, are independent of the initial y -coordinate.

We now go through the different dynamic states depicted in Fig. 5.1. The most trivial state is represented by the turquoise filled pentagon symbols in Fig. 5.1(a). They indicate a *passive straight motion*. In the absence of any external flow field, a particle in this state is motionless and has a circular shape. When the shear flow is switched on, the particle is elongated due to the elongational contribution from the flow field. Nevertheless, its active self-propulsion velocity remains zero, $v = 0$, so that it is just passively advected with the flow field. We do not include plots of these trivial trajectories in Fig. 5.1.

Next, a particle that moves straight in a condition without shear flow continues to move straight in the presence of shear flow at low shear rates $\dot{\gamma}$. It features a time-independent steady state of deformation. Such a situation is marked by the green open pentagons in the phase diagram Fig. 5.1(a) and shown in Fig. 5.1(b) for $\kappa_1 = -0.5$ and

$\dot{\gamma} = 0.1$. The real-space trajectory is only bended a little because of the advection in x -direction with the fluid flow that increases in the y -direction due to the shear geometry. Since $v \neq 0$, we term this type of motion an *active straight motion* in this chapter. We note from the line $\kappa_1 = 0.1$ in the phase diagram Fig. 5.1(a) that with increasing shear rate $\dot{\gamma}$ a transition from the passive to active straight motions can be induced. Interestingly, the phase behavior is reentrant, and we again observe the passive straight motion at very high shear rates. The reason for this behavior is that the deformation $\mathbf{S}$ depends on the shear rate and thus is induced via the shear flow as in Eq. (5.6). They in turn couple to the relative velocity $\mathbf{v}$ in Eq. (5.5) and at intermediate shear rates induce the active self-propulsion.

If a particle undergoes a circular motion when the shear is absent, it exhibits what we call a *cycloidal I motion* under a small nonzero shear flow as indicated by the red open squares in Fig. 5.1(a). In this state, a particle moves on a cycloidal trajectory with $v \neq 0$ and with its deformation axes rotating as depicted in Figs. 5.1(c) and (d), both for $\kappa_1 = -0.9$ and $\dot{\gamma} = 0.1$. Both clockwise (c) and counter-clockwise (d) rotation are possible. Whether clockwise or counter-clockwise rotation appears during the cycloidal I motion generally depends on the initial conditions. At higher shear rates close to the stability boundary of the cycloidal I motion, however, cycloidal I motion of counter-clockwise rotation becomes unstable first, before the one with clockwise rotation. This is because the rotational contribution of the shear flow is oriented in clockwise direction and breaks the rotational symmetry of space. However, the effect occurs within a thinner parameter region than the grid size in Fig. 5.1(a) resolves. Therefore we do not mark this region in the phase diagram Fig. 5.1(a).

So far, we have only discussed types of motion that result directly as a generalisation of the types of motion found for vanishing flow field $\dot{\gamma} = 0$ [110, 112]. Quite contrarily, the following types of motion are qualitatively different and newly observed in the presence of the shear flow.

When the cycloidal I motion has become unstable at high shear rates, the particle exhibits a *winding I motion*. The corresponding narrow region in the phase diagram Fig. 5.1(a) is marked by the purple filled triangles. It is located between the cycloidal I motion and the active straight motion. For this winding I motion, the long axis of the particle does not make a full rotation in the laboratory frame. It only oscillates in time around the velocity vector, as shown in Fig. 5.1(e) for $\kappa_1 = -0.7$ and $\dot{\gamma} = 0.08$. In particular, the trajectory in θ_2 - ϕ space exhibits a closed loop indicating an oscillation. In contrast to the active straight motion, both the relative velocity and the deformations of the particle are time-dependent.

Finally, at high shear rates, also the active straight motion becomes unstable, and a *cycloidal II motion* appears. It is indicated by the gray filled squares in Fig. 5.1(a) and further characterised in Fig. 5.1(f) for $\kappa_1 = -0.1$ and $\dot{\gamma} = 2$. Again the centre of mass of the particle draws a cycloidal trajectory in real space. However, as can be seen from the trajectory in θ_2 - ϕ space, the value of θ_2 stays close to zero with only small oscillations around it. Thus, in contrast to the cycloidal I motion, the elongation axis of deformation remains approximately horizontal for all times.

5.4 Full dynamics

In the previous two sections, we considered simplified special cases of the dynamic equations (5.4)–(5.7) to identify the basic states of motion. First we neglected deformations in Section 5.2, we then excluded active contributions from the rotational motion in Section 5.3. Nevertheless, the dynamics in both cases was already quite complex. This complexity is increased even further when we now investigate the full active dynamics. For example qualitatively new quasi-periodic and chaotic states arise.

We use the same methods and the same parameter values as in the previous section to study the full set of dynamic equations (5.4)–(5.7). The only difference is that now the active rotation of the particle is taken into account. They are induced by setting ζ to a positive value, $\zeta = 1.5$ in our current case, in Eq. (5.7). Since the rotational symmetry of space is broken by the shear flow given by Eq. (5.8) with $\dot{\gamma} \neq 0$, we distinguish between the following two cases. First, we consider the clockwise active rotation of the particle, after that the counter-clockwise active rotation. The rotational part of the shear flow itself is oriented in the clockwise direction for $\dot{\gamma} > 0$. Our results are again presented in terms of the quantities introduced in Eqs. (5.14), (5.34), and (5.35).

5.4.1 Clockwise active rotation

Without an externally imposed shear flow, i.e. for $\dot{\gamma} = 0$, the situation with the active rotation has been recently investigated [111, 112]. For the parameters that we have chosen in this chapter, two types of motion have been found in the absence of the shear flow: circular and quasi-periodic motions. We repeat these results on the left border of our phase diagram Fig. 5.2(a) in the column $\dot{\gamma} = 0$. There, with increasing self-propulsion strength, i.e., decreasing κ_1 , the circular motion is reentrant [111, 112].

With the shear flow now turned on and the active rotation in clockwise direction, the circular motion changes to the corresponding cycloidal I motion that was already obtained in the previous section and characterised in Fig. 5.1(c) for $\zeta = -0.1$. It covers a major part of our phase diagram Fig. 5.2(a) and is indicated by the red open squares. A cycloidal trajectory naturally results, when advection due to the flow is superimposed to a circular motion.

Next, the black crosses in the phase diagram in Fig. 5.2(a) mark a *quasi-periodic motion*. It occurs at intermediate self-propulsion strengths κ_1 . Interestingly, this type of motion is suppressed with increasing shear-rate $\dot{\gamma}$. We further characterise it in Fig. 5.2(b) for $\kappa_1 = -0.5$ and $\dot{\gamma} = 0.1$. Obviously, the motion is not simply periodic as evident from the real-space trajectory and from the trajectories indicated in the θ_2 - ϕ and s_2 - ψ phase spaces in red. However, it is quasi-periodic and not chaotic, because the return maps give discrete closed loops as shown in the second column of Fig. 5.2(b). The difference between the quasi-periodic motion in the absence of the shear flow and the one in the presence of the shear flow is simply that the particle stays within a finite area in the former case while in the latter case it escapes over time in the positive or negative x -direction.

When the shear rate $\dot{\gamma}$ is increased, several new types of motion are found that we

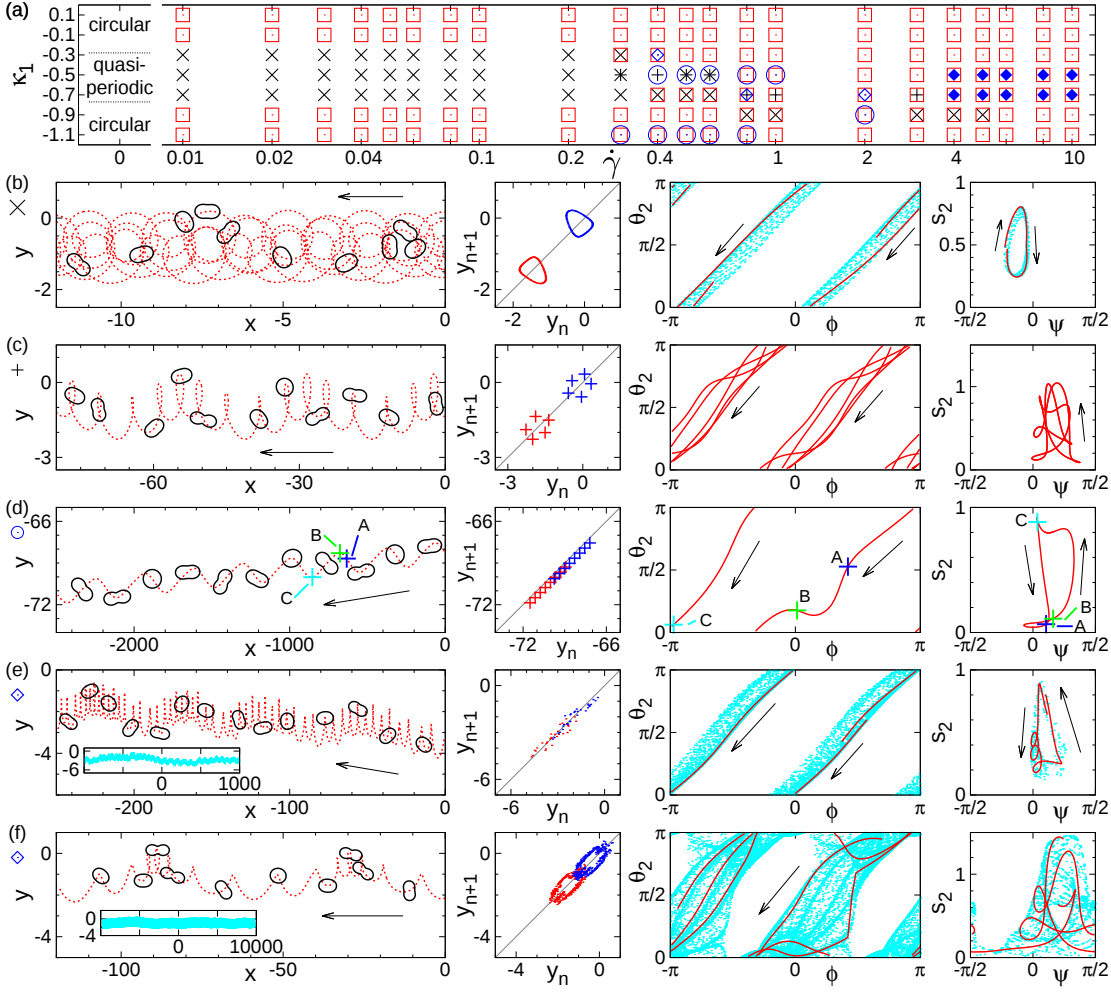


Figure 5.2: (a) Dynamical phase diagram and (b)–(f) trajectories in real space (1st column), return maps (2nd column), attractors in θ_2 - ϕ space (3rd column) as well as in s - ψ space (4th column) of the typical dynamical motions, obtained by solving Eqs. (5.4)–(5.7) numerically in two dimensions for clockwise active rotation ($\zeta = 1.5$); (b) *quasi-periodic motion* for $\kappa_1 = -0.5$ and $\dot{\gamma} = 0.1$ indicated by the black crosses in panel (a); (c) *periodic motion* for $\kappa_1 = -0.7$ and $\dot{\gamma} = 1$ marked by the black plus symbols in panel (a); (d) *winding II motion* for $\kappa_1 = -0.5$ and $\dot{\gamma} = 0.8$ identified by the blue open circles in panel (a); (e) and (f) *chaotic motions* for $\kappa_1 = -0.3$ and $\dot{\gamma} = 0.4$ as well as for $\kappa_1 = -0.7$ and $\dot{\gamma} = 2$, respectively, marked by the purple open diamonds in panel (a). Arrows in panels (b)–(f) show the directions of motion. Insets in panels (e) and (f) show the corresponding trajectories over longer time intervals. The trajectories in θ_2 - ϕ and s_2 - ψ phase space in panels (b), (e), and (f) are indicated in turquoise with short-time trajectories in red. Red open squares stands for the *cycloidal I motion* as already characterised in Fig. 5.1(c) for $\zeta = -0.1$. The blue filled diamonds in panel (a) represent an *undulated cycloidal I motion*, which is further illustrated by Fig. 5.3(c).

have not observed before. Interestingly, all of them are sensitive to the initial conditions. We find a coexistence of at least two types of motion at every point of the phase diagram that we investigated for these new dynamic states, which leads to the superposition of the symbols in Fig. 5.2(a).

First, at higher shear rates, a *periodic motion* that cannot be observed at low shear rates is found at some positions in the phase diagram. This dynamic state is marked by the black plus symbols in Fig. 5.2(a) and further illustrated in Fig. 5.2(c) for $\kappa_1 = -0.7$ and $\dot{\gamma} = 1$. The real-space trajectory appears as a commensurately modulated cycloid. We can distinguish this kind of motion from the quasi-periodic motion by the return map in the second column of Fig. 5.2(c), where thousands of measured trajectory extrema condense on ten discrete points in contrast to the closed loop object in Fig. 5.2(b). There are even some coexistence points of periodic and quasi-periodic motion in the phase diagram, induced by different initial conditions.

Next, in analogy to the winding I motion of the previous section, a *winding II motion* is identified at the positions of the blue open circles in the phase diagram Fig. 5.2(a). We characterise it in Fig. 5.2(d) for $\kappa_1 = -0.5$ and $\dot{\gamma} = 0.8$. Since the particle in real space continuously descends in y -direction, the discrete points in the return map descend along the diagonal. The winding II motion can easily be distinguished from its counterpart, the winding I motion in Fig. 5.1(e), by the trajectory in θ_2 - ϕ phase space. When observed from the laboratory frame, the particle features a full rotation of its long axis of deformation $\mathbf{S}$ in the winding II state, while only oscillations of this long axis occur in the winding I state. To facilitate the connection between the real- and phase-space trajectories in Fig. 5.2(d), we marked corresponding points by the capital letters “A”, “B”, and “C”. We found a three-state coexistence region including the winding II motion, the periodic motion, and the quasi-periodic motion in the phase diagram Fig. 5.2(a) around the point $\kappa_1 = -0.5$ and $\dot{\gamma} = 0.6$.

Most interestingly, we now also find *chaotic states* of the dynamic behavior of our single deformable active particle subjected to a linear shear flow. In the phase diagram Fig. 5.2(a) they are marked by the blue open diamonds. Figures 5.2(e) and (f) show the characteristics of two chaotic dynamic states for $\kappa_1 = -0.3$ and $\dot{\gamma} = 0.4$ as well as for $\kappa_1 = -0.7$ and $\dot{\gamma} = 2$, respectively. The inset figures in the real-space trajectory plots in the first column of Figs. 5.2(e) and (f) depict the trajectory over longer time intervals. Closer inspection shows that the attractors in the θ_2 - ϕ and s_2 - ψ phase spaces of Fig. 5.2(e) are similar to the ones of the quasi-periodic motion in Fig. 5.2(b). However, the return maps are different enough to distinguish these two separate types of motion: the return map of the quasi-periodic motion forms a simple closed loop, while that of the chaotic motion in Fig. 5.2(e) is dispersed around the diagonal $y_{n+1} = y_n$. Likewise, we can distinguish the chaotic motion in Fig. 5.2(f) from the undulated cycloidal I motion discussed below in Fig. 5.3(c) via their return maps, although the attractors in θ_2 - ϕ space and s_2 - ψ space are similar.

At large shear rates $\dot{\gamma}$ and intermediate self-propulsion strengths κ_1 , another dynamic state was observed. It is marked by the blue filled diamonds in the phase diagram Fig. 5.2(a) and we call it an *undulated cycloidal I motion*. Since it also appears in the case of counter-clockwise active rotation of the particle, we discuss it below together

with the dynamic states observed in that case.

5.4.2 Counter-clockwise active rotation

Finally, we analyse the case of the counter-clockwise active rotation of the active particle, i.e. the active rotation in the direction opposite to that of the rotational part of the shear flow. Without the shear flow at $\dot{\gamma} = 0$, the rotational symmetry in space is not broken, and the dynamical states of clock- and counter-clockwise rotation are identical (except for the sense of rotation).

At low shear rates, the dynamics for both senses of rotation are still similar as can be inferred when comparing the corresponding phase diagrams Figs. 5.2(a) and 5.3(a) for low values of $\dot{\gamma}$. Again, a cycloidal I motion appears for both high and low self-propulsion strengths κ_1 . Likewise, a quasi-periodic motion emerges at intermediate self-propulsion strengths κ_1 . They are marked by the red open squares and black crosses in the phase diagram Fig. 5.3 and were discussed in Figs. 5.1(d) and 5.2(b), respectively. Increasing the shear rate $\dot{\gamma}$, the quasi-periodic motion becomes unstable in favor of the cycloidal I motion. Also the periodic motion, indicated by the black pluses and previously characterised in Fig. 5.2(c), as well as the winding II motion, marked by the blue open circle and previously depicted in Fig. 5.2(d), are recovered. Coexistence of different dynamic states again occurs and is shown by the superposition of different symbols in the phase diagram Fig. 5.3(a).

Interestingly, at large shear rates $\dot{\gamma} \gtrsim 1$, we observe the active-straight motion at all investigated self-propulsion strengths κ_1 . It is indicated in the phase diagram Fig. 5.3(a) by the green open pentagons and was previously discussed in Fig. 5.1(b). The origin of the emergence of the active straight motion at these shear rates can be easily understood. It appears when the active rotation in the counter-clockwise direction and the passive rotation due to the external flow in the clockwise direction balance each other.

At still larger shear rates $\dot{\gamma}$, this balance is no longer maintained and different types of motion appear. At high self-propulsion strength, i.e., small $\kappa_1 < 0$, the particle next undergoes a *winding III motion* as denoted by the blue open downward triangles in the phase diagram Fig. 5.3(a). This motion is characterised in Fig. 5.3(b) for $\kappa_1 = -0.9$ and $\dot{\gamma} = 4$. In contrast to the winding I and winding II motions in Figs. 5.1(e) and 5.2(d), respectively, the angle θ_2 as viewed from the laboratory frame always remains of small magnitude with values close to zero. This means that the particle always remains elongated along the horizontal direction. Only small oscillations of the long axis of deformation occur that are due to the competition between the active rotation in the counter-clockwise direction and the clockwise rotation induced by the shear flow. In Fig. 5.3(b), capital letters “A”, “B”, and “C” are again used to mark corresponding points along the trajectories in real space, in θ_2 - ϕ phase space, and in s_2 - ψ phase space.

In Section 5.3 we have already found a dynamical mode that features an almost horizontal elongation of the particle at all times. It was the cycloidal II motion, obtained without active rotation, and depicted in Fig. 5.1(f). Indeed, we find this type of motion again when increasing the shear rate $\dot{\gamma}$ from the winding III motion at high self-propulsion strengths, i.e., small $\kappa_1 < 0$. In addition to that, it is also the dominant dynamical mode

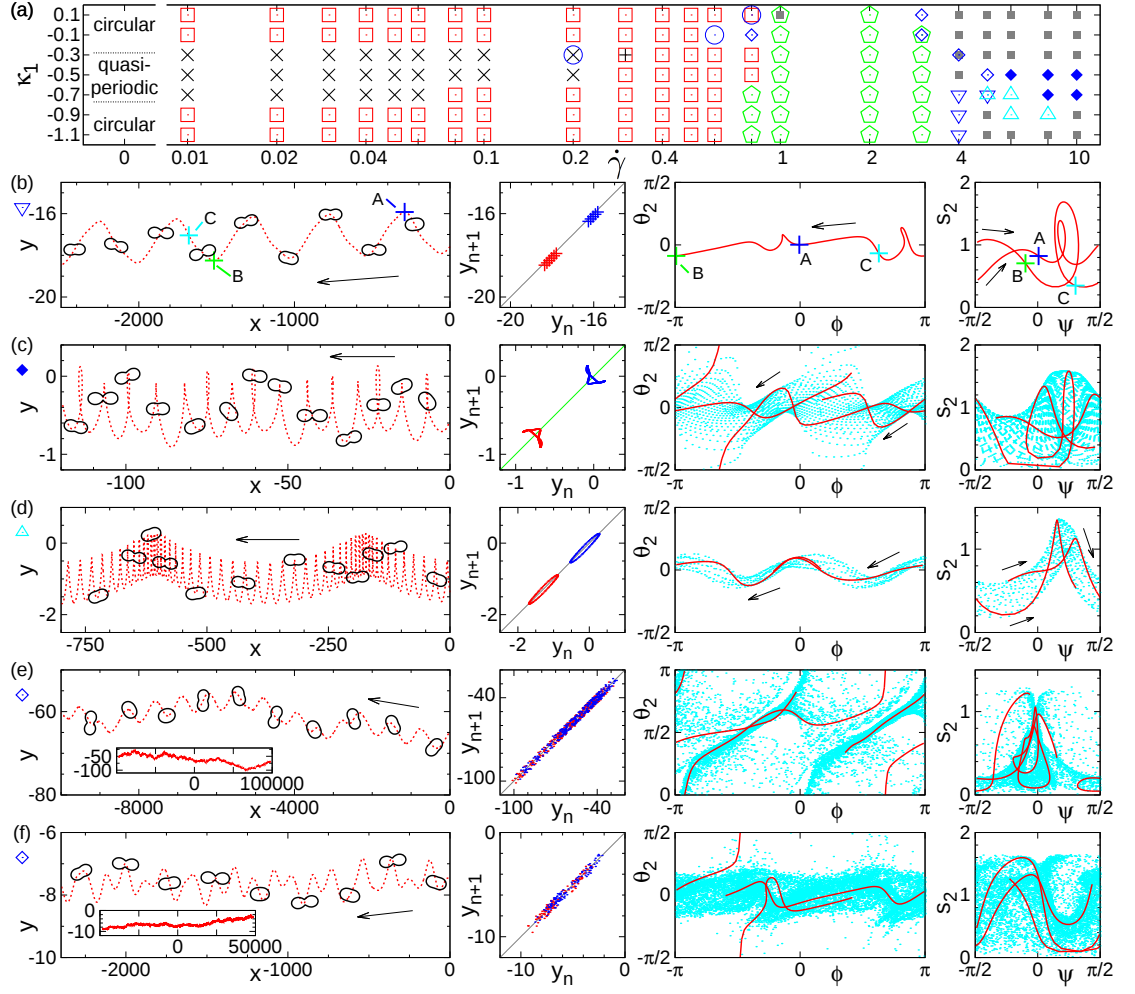


Figure 5.3: (a) Dynamical phase diagram and (b)–(f) trajectories in real space (1st column), return maps (2nd column), attractors in θ_2 - ϕ space (3rd column) as well as in s_2 - ψ space (4th column) of the typical dynamical motions, obtained by solving Eqs. (5.4)–(5.7) numerically in two dimensions for counter-clockwise active rotations ($\zeta = 1.5$); (b) *winding III motion* for $\kappa_1 = -0.9$ and $\dot{\gamma} = 4$ indicated by the blue open downward triangles in panel (a); (c) *undulated cycloidal I motion* for $\kappa_1 = -0.5$ and $\dot{\gamma} = 6$ specified by the blue filled diamonds in panel (a); (d) *undulated cycloidal II motion* for $\kappa_1 = -0.9$ and $\dot{\gamma} = 6$ marked by the turquoise open upward triangles in panel (a); (e) and (f) *chaotic motions* for $\kappa_1 = -0.1$ and $\dot{\gamma} = 0.8$ as well as for $\kappa_1 = -0.3$ and $\dot{\gamma} = 4$, respectively, indicated by the blue open diamonds in panel (a). Arrows in panels (b)–(f) show the directions of motion. Insets in panels (e) and (f) show the corresponding trajectories over longer time intervals. The trajectories in θ_2 - ϕ and s_2 - ψ phase space in panels (c)–(f) are indicated in turquoise with short-time trajectories in red. The dynamical states corresponding to the other symbols in panel (a) that are not further characterised in panels (b)–(f) have already been explained in Figs. 5.1 and 5.2.

at large shear rate $\dot{\gamma}$ but small self-propulsion strength, i.e., large $\kappa_1 < 0$. We indicate it again by the gray filled squares in Fig. 5.3(a).

Apart from the cycloidal I and II motions, depicted previously in Figs. 5.1(c) and (d) as well as in Fig. 5.1(f), respectively, there are two other types of cycloidal motions. One of them is the undulated cycloidal I motion that has already been found for the clockwise active rotation. It is marked by the blue filled diamonds in the phase diagrams in Figs. 5.2(a) and 5.3(a). We now further characterise it in Fig. 5.3(c) for $\kappa_1 = -0.5$ and $\dot{\gamma} = 6$. An undulation of the cycloidal amplitude is apparent from the real-space trajectory as well as from the return map. As can be seen in θ_2 - ϕ phase space, the long axis of deformation makes a full rotation in the laboratory frame.

The other further cycloidal type is the new *undulated cycloidal II motion* that we find only for the particle with the counter-clockwise active rotation and that we mark by the turquoise open upward triangles in Fig. 5.3(a). We illustrate this dynamical mode in Fig. 5.3(d) for $\kappa_1 = -0.9$ and $\dot{\gamma} = 6$. In contrast to the undulated cycloidal I motion, there is no full rotation of the long axis of deformation in the laboratory frame as becomes obvious in θ_2 - ϕ phase space.

Again we also observe chaotic motions, which are represented by the blue open diamonds in Fig. 5.3(a). Characteristics of these chaotic motions are displayed in Figs. 5.3(e) and (f) for $\kappa_1 = -0.1$ and $\dot{\gamma} = 0.8$ as well as for $\kappa_1 = -0.3$ and $\dot{\gamma} = 4$, respectively. A qualitative difference between the two depicted chaotic motions becomes obvious from the plots in phase space. While in the first case of Fig. 5.3(e) the long axis of deformation of the particle tends to rotate together with the velocity direction, it has a tendency to remain horizontal in the second case of Fig. 5.3(f). Both tendencies can be inferred from the turquoise bands in the θ_2 - ϕ plots. Generally, we find that the trajectories in phase space in Figs. 5.3(e) and (f) are more delocalised than for the chaotic states of the clockwise rotation that we have illustrated in Figs. 5.2(e) and (f).

5.5 Summary and Conclusions

In this chapter, we have investigated the dynamics of a deformable active particle in an external flow field. For this purpose, we have considered a soft deformable particle with two types of activity. One is spontaneous propulsion and the other one is spontaneous rotation. The deformation of the particle is described by a symmetric traceless tensor variable, and the rotation by an antisymmetric tensor variable. Further variables are the position of the center of mass and its relative velocity with respect to the flow. The externally imposed flow field is included in terms of its elongational and rotational impacts. Using symmetry arguments, we derive coupled dynamic equations for all of these variables. Our equations reduce to known models in the two limits of vanishing the external flow and vanishing particle deformability. On the one hand, in the limit of vanishing flow field, we reproduce the previous results of Refs. [111, 112]. On the other hand, for vanishing particle deformability, we obtain an approximate analytical solution for a linear shear flow that is consistent with the previous investigations [144].

For an externally imposed linear shear flow, various types of motion arise as numerical

solutions of the full set of dynamical equations including active straight motion, periodic motions, motions on regular and undulated cycloids, winding motions, as well as quasi-periodic and chaotic motions induced at high shear rates. In order to characterise and distinguish these dynamical states, we have analysed and categorised them via their trajectories, corresponding return maps, as well as their attractors in phase space. Also the two situations of clockwise and counter-clockwise rotation with respect to the rotational direction of the shear flow are distinguished and lead to partially different results, in particular at high shear rates.

Our predictions can be verified in experiments on self-propelled droplets exposed to a shear flow. For instance, in some experiments [38, 40] self-propelled droplets on liquid-air interfaces can be exposed to linear shear fields by putting the carrier liquid between two parallel confining walls that move alongside into opposite directions. This induces an approximately planar linear shear gradient at the surface of the carrier liquid, if the liquid container is sufficiently deep. Since the motion of the droplets is confined to the liquid-air interface, the geometry is quasi-two dimensional. Using this experimental setup, it is in principle possible to verify the phenomena predicted by our analysis.

Future studies should address several extensions of our model: first of all, different prescribed flow fields can be explored using our equations. Most noticeable examples include a Poiseuille flow [145] or an imposed vorticity field. We expect again a manifold of different types of motion in these flow fields presuming that the different flow topologies will induce different types of motion. The next step is to extend our analysis to a finite concentration of particles and to include steric interactions between them. This is a complex problem, which is already very difficult for rigid self-propelled particles [70, 71, 73, 141, 152–156]. Another step is to extend the current analysis of the model to three spatial dimensions. In a previous study, some of us demonstrated that —without shear flow— a particle can exhibit additional qualitatively different types of motion when comparing a three- to a two-dimensional setup [112]. In the case without an external flow, these were additional helical and superhelical types of motion [112]. Thus we expect that further new types of dynamics can arise in three dimensions when the shear flow is included. Finally one could access the dynamics of propelled vesicles by using our analysis as a starting point. Here one should impose the constraints of constant volume and constant surface area of the deformable particle. The dynamics of passive vesicles in shear flow have been explored quite extensively in recent years [157, 158] with various specific effects like tank-treading motion, lifting [159, 160], wrinkling [161], tumbling and swinging [162, 163]. It would indeed be interesting to generalise all these effects to self-propelled vesicles.

Chapter 6

Active deformable particle in a swirl

As we have discussed in the previous Chapter 5, both biological and artificial active particles in natural situations suffer from their surroundings, such as gravity, gradient of chemical concentrations, and walls. Therefore, it is important to study how the existence of external fields changes the dynamics of active particles. Besides, for many applications it is of key relevance to tune and control the motion of artificial and biological active particles [1, 5, 91] by external influences like confinement [140, 141, 164–167], solvent flow [144, 145, 168, 169], or a magnetic field [170]. This can be exploited to construct motors and machines on the microscale [171–173] and artificial muscles [174], to mention just a few examples. In particular the motion of self-propelled particles in externally prescribed flow fields gives rise to significant changes in their trajectories as shown by recent studies in planar Couette [144] and Poiseuille flow geometry [145, 168, 169].

Astonishingly the motion of an active particle in a swirl has never been considered except our study [115], although swirl flows occur quite naturally in many situations, including turbulence. Here we address this problem and augment it by possible deformations of the particle that couple to the solvent flow. Using a theoretical description introduced in the previous Chapter 5 [114], we derive equations of motion for an active deformable particle in a swirl. The setup of a swirl is similar to that of a scattering geometry and possesses therefore an analogy to the classical Kepler and Rutherford problem. In particular, one can discriminate between the two basic dynamic events of capturing and scattering. In the former, the particle is attracted by the swirl and cannot escape from it afterwards, while in the latter it escapes from the eddy by its own self-propulsion. In fact, the two events of capturing, which possibly leads to death, and scattering, corresponding to a successful escape and survival, depend on the impact parameter and the relative orientation of the active deformable particle with respect to the flow direction. We address this problem in terms of active matter. In order to discriminate between these two results, we perform a theoretical stability analysis of the steady-state solutions as well as a numerical simulation of the corresponding equations of motion.

This chapter is organised as follows. In the next section, the time-evolution equations of an active deformable particle in a swirl flow are described. We discuss the steady-state solutions and their stability in Section 6.2. Scattering and capturing dynamics, which actually constitute the central topic of this chapter, are considered in Section 6.3.

The effect of the stochastic fluctuations on the scattering and capturing events are also considered briefly. Section 6.4 is devoted to the summary and conclusions of this chapter. Finally, details of the analytical calculations carried out in Section 6.2 are explained in the Appendix 6.A.

The argument developed in this chapter is one of the main issues of this thesis and is based on the study carried out by the present author published in Ref. [115].¹

6.1 Time-evolution equations

We introduce the model equations for an active deformable particle in a swirl flow. We consider a two-dimensional environment and denote the fluid flow field as $\mathbf{u}(x, y)$. Our simple vortex flow (swirl) is given by

$$\mathbf{u}(x, y) = \left(\mu \frac{-y}{x^2 + y^2}, \mu \frac{x}{x^2 + y^2} \right), \quad (6.1)$$

where μ sets the strength of the vortex. It describes a rotational flow around a swirl center. Naturally, the swirl center defines the origin of our coordinate frame. A flow potential exists for this type of fluid flow such that $\mathbf{u}(x, y) = -\nabla U(x, y)$, where $U(x, y) = \mu \arctan(x/y)$. Consequently $\nabla \times \mathbf{u} = \mathbf{0}$, which implies that the fluid flow does not contain a local rotational contribution. On the other hand, there exists an elongational contribution of the swirl flow, which is characterised by the symmetric tensor $\mathbf{A}$:

$$\mathbf{A} = \begin{bmatrix} \mu r^{-2} \sin 3\eta & -\mu r^{-2} \cos 2\eta \\ -\mu r^{-2} \cos 2\eta & -\mu r^{-2} \sin 2\eta \end{bmatrix}. \quad (6.2)$$

For a simple active particle, two basic kinds of activity can generally be distinguished: a spontaneous translational motion (self-propulsion), and a spontaneous spinning motion (active rotation). Here, for simplicity, we take into account only the spontaneous translational motion, i.e. self-propulsion. By using the time-evolution equations for active deformable particles in a flow field derived from symmetry argument in the previous Chapter 5, the equations of motion for an active deformable particle in a fluid flow field $\mathbf{u}$ can then be introduced as [115]

$$\frac{dx_i}{dt} = u_i + v_i, \quad (6.3)$$

$$\frac{dv_i}{dt} = -\kappa_1 v_i - a_0 (v_k v_k) v_i - a_1 S_{ik} v_k, \quad (6.4)$$

$$\frac{dS_{ij}}{dt} = -\kappa_2 S_{ij} + b_1 \left[v_i v_j - \frac{\delta_{ij}}{2} (v_k v_k) \right] + \nu_1 \left[A_{ij} - \frac{\delta_{ij}}{2} A_{kk} \right], \quad (6.5)$$

where δ_{ij} is the Kronecker delta and summation over repeated indices is implied.

¹ The contents of this chapter are same as those in the publication by the author of this thesis in Ref. [115]. All the figures, Figs. 6.1, 6.2, 6.3, 6.4, 6.5, 6.6, and 6.7, are newly produced for this thesis.

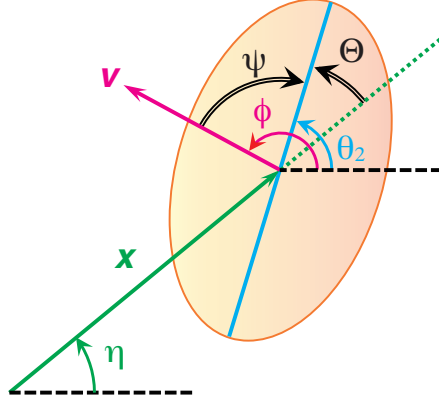


Figure 6.1: Variables characterising the orientational degrees of freedom of an elliptically-deformable active particle when viewed from the laboratory frame (schematic).

The variables in the above equations are as follows. $\mathbf{x} = (x_1, x_2)$ represents the position of the center of mass of the particle. It is parameterized as

$$\mathbf{x} = (r \cos \eta, r \sin \eta) \quad (6.6)$$

in polar coordinates.

When viewed from the laboratory frame, the active particle in total moves with the velocity $\mathbf{u} + \mathbf{v}$. In this expression, $\mathbf{u}$ is the imposed flow velocity of the fluid fixed by Eq. (6.1), while $\mathbf{v}$ is the active velocity of the particle measured with respect to its fluid environment. We parameterize $\mathbf{v}$ as

$$\mathbf{v} = (v \cos \phi, v \sin \phi). \quad (6.7)$$

In a lowest-order approach, we take into account elliptic deformations of the particle and describe them by a traceless second-order symmetric tensor $\mathbf{S}$. The components of $\mathbf{S}$ are parameterized as

$$\mathbf{S} = \begin{bmatrix} s_2 \cos 2\theta_2 & s_2 \sin 2\theta_2 \\ s_2 \sin 2\theta_2 & -s_2 \cos 2\theta_2 \end{bmatrix}. \quad (6.8)$$

Here s_2 characterises the degree of elliptic deformation, while θ_2 measures the orientation of the symmetry axis of elliptic deformation viewed from the laboratory frame. See Fig. 6.1 for the assignment of the angles η , ϕ , and θ_2 .

We briefly explain the meaning of each term in Eqs. (6.4)–(6.5). On the right-hand side of Eq. (6.4), the first two terms with the coefficients κ_1 and a_0 are the crucial one for active particle. It describes self-propulsion with a net non-vanishing velocity of active particle in the case of $\kappa_1 < 0$. On the contrary, we do not include active deformations of the particle. It rather tends to relax back to the undeformed state. This is implied by the contribution with the coefficient $\kappa_2 > 0$ in Eq. (6.5).

The terms with the coefficients a_1 and b_1 represent the leading-order coupling terms between the active velocity $\mathbf{v}$ and the deformation $\mathbf{S}$. Accordingly, self-propulsion can

lead to shape changes, whereas in turn deformations can influence the propulsion direction and the translation speed. One important result is that increased deformations lead to curved trajectories [110]. Without the fluid flow, a bifurcation from a straight motion to a circular motion is found from Eqs. (6.4) and (6.5) at a critical value $\kappa_1 = \kappa_1^c$. These coupling terms also influence the relation between the direction of the elongation and that of the active velocity. If $a_1 > 0$ and $b_1 > 0$, the longitudinal axis of the elliptical deformation tends to be parallel to the propulsion velocity (“parallel case”) [110]. In contrast, if $a_1 < 0$ and $b_1 < 0$, the two directions tend to be perpendicular to each other (“perpendicular case”) [110].

Finally, the last term on the right-hand side of Eq. (6.5) represents the elongational contribution of the flow on the shape of the particle. Depending on the coefficient ν_1 , the elongational part of the fluid flow can lead to stretching deformations of the deformable particle.

6.2 Steady-state solutions

The swirl flow in Eq. (6.1) features a rotational symmetry. One therefore expects that circular steady-state solutions of closed circular loops exist, at least for passive particles. For rigid spherical passive particles, implying $\kappa_1 > 0$ and $\kappa_2 \rightarrow \infty$, Eqs. (6.3)–(6.5) reduce to $d\mathbf{x}/dt = \mathbf{u}$, $\mathbf{v} = \mathbf{0}$, and $\mathbf{S} = \mathbf{0}$. Thus these objects are simply advected by the fluid flow on circles around the vortex center. The stability of the circular motion of any radius is marginal, with the radius only determined by the initial conditions. This section concerns how deformability and self-propulsion change this result. To this end, we develop stability analysis of the steady-state solutions of Eqs. (6.3)–(6.5).

6.2.1 Passive circular motion

We first consider a passive deformable particle, i.e. one that does not propel spontaneously. Consequently it is simply convected by the fluid flow, and the active velocity with respect to the surrounding fluid vanishes, $\mathbf{v} = \mathbf{0}$. Nevertheless, the particle can be deformed by the elongational component of the flow field.

Under these assumptions, we investigate the steady-state solutions of Eqs. (6.3)–(6.5). It turns out that the only remaining orientational degree of freedom is the relative angle ψ between the deformation axis and the position vector of the particle, i.e. $\psi = \theta_2 - \eta$. As explained in more detail in the Appendix 6.A, we find circular trajectories of fixed radius $r = r_0$ characterised by

$$\tan 2\psi = \frac{\kappa_2 r_0^2}{2\mu}, \quad (6.9)$$

$$s = -\frac{\nu_1}{\kappa_2} \mu r_0^{-2} \sin 2\psi. \quad (6.10)$$

An illustrative picture of these trajectories is given by a permanently deformed particle, anchored under the angle ψ to the pointer of a working clock. We refer to this situation as *passive circular motion*.

The set of these solutions are marginally stable for

$$\kappa_1 > \begin{cases} 0 & \text{for } r_0 < r_c \\ \kappa_1^\dagger & \text{for } r_0 \geq r_c \end{cases} \quad (6.11)$$

with the constants r_c and $\kappa_1^\dagger$ defined as

$$r_c = (2|\mu|)^{1/2} \left\{ (a_1\nu_1)^2 - \kappa_2^2 \right\}^{-1/4}, \quad (6.12)$$

$$\kappa_1^\dagger = \frac{2\mu^2}{r_0^2 r_c^2} \left\{ \frac{(r_0^4 - r_c^4)}{\kappa_2^2 r_0^4 + 4\mu^2} \right\}^{1/2} > 0. \quad (6.13)$$

The detailed derivation of this stability condition is given in the Appendix 6.A. The stability is marginal with respect to the radial direction and asymptotic with respect to the other degrees of freedom.

Equations (6.11)–(6.13) imply that for increasing stiffness of the particle the stability range of the passive circular motion increases. This can be seen as follows. Increasing stiffness corresponds to increasing magnitude of $\kappa_2 > 0$. As κ_2 approaches $|a_1\nu_1|$ from below, the value of r_c diverges. Thus $\kappa_2 \geq |a_1\nu_1|$, the condition for κ_1 in Eq. (6.11) extends to the full range of $\kappa_1 > 0$. This corresponds to the natural requirement that a passive particle suffers from the friction with its fluid environment, with $\kappa_1 > 0$ setting the friction parameter. Therefore, in this case, circular steady-state trajectories of all radii are marginally stable.

Coming back to passive deformable particles, we checked our analytical predictions by numerically solving the equations of motion Eqs. (6.3)–(6.5). In the following, we always employed a fourth-order Runge-Kutta method of time increment $\delta t = 10^{-3}$ and checked our results using still finer time steps. Here, we initialised the system by circular particles placed at different distances from the vortex center.

Figure 6.2 shows corresponding numerical results for the system parameters chosen as $\kappa_2 = 0.5$, $a_1 = b_1 = -1$, $\nu_1 = 1$, and $\mu = 1$, and hence, $\kappa_2 < |a_1\nu_1|$ is satisfied. This implies soft deformable particles. Indeed we find our analytical results confirmed. The solid (blue) line marks the stability limit derived in Eqs. (6.11) and (6.13). Circular trajectories of radius r_0 with a value of κ_1 above this line are stable. On the contrary, if we initialise trajectories with $\kappa_1 > 0$ below the solid stability line (i.e. within the “hump” region in Fig. 6.2), the system is expelled from that area as indicated by the horizontal arrows. Most of the dense points in Fig. 6.2 on both sides of the hump follow from such expelled systems. As we can see, the expelled systems typically overshoot the stability line until they finally get stabilised. We checked numerically that the results are qualitatively the same when $a_1 = b_1 = +1$, as it is predicted from our theoretical analysis.

6.2.2 Active circular motion of deformable particles

We now turn to steady-state active motions with $\mathbf{v} \neq \mathbf{0}$ for $\kappa_1 < 0$. As noted above, in the absence of the fluid flow a straight motion is obtained for $\kappa_1^c < \kappa_1 < 0$ and a circular

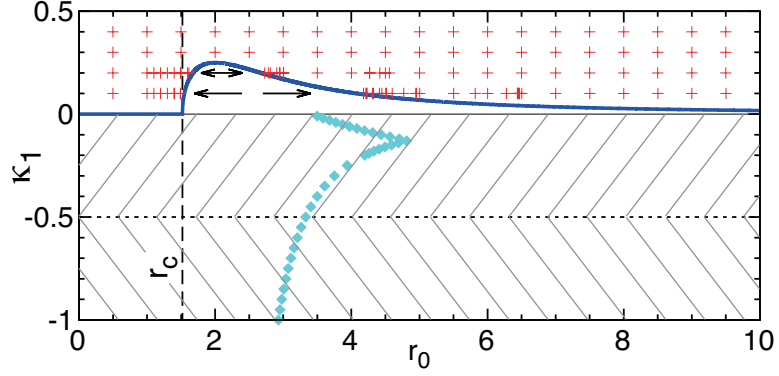


Figure 6.2: Radius r_0 of a stable circular motion for soft deformable particles with the perpendicular configuration. $\kappa_1 > 0$ characterises the friction for passive particles (plusses), whereas $\kappa_1 < 0$ measures the self-propulsion speed of active particles (cyan diamonds). The vertical dashed line indicates the value of the radius r_c defined in Eq. (6.12). The solid blue line gives the stability range of circular trajectories for deformable passive particles following Eqs. (6.11) and (6.13). Passive systems initialised in the “hump” region are horizontally expelled from that area as indicated by the arrows. Active particles perform different types of motion, depending on the initial conditions: an active circular motion (cyan diamonds) or an escape (not indicated) for $\kappa_1^c < \kappa_1 < 0$ (upper hatched area); An active circular motion (cyan diamonds) or a lunar motion (not indicated) for $\kappa_1 < \kappa_1^c$ (lower hatched area). The system parameters are set to $\kappa_2 = 0.5$, $a_1 = b_1 = -1$, $\nu_1 = 1$, and $\mu = 1$. For these parameters, the bifurcation threshold between the straight motion to the circular motion in the absence of the flow is given by $\kappa_1^c = -0.5$.

motion for $\kappa_1 < \kappa_1^c$, with κ_1^c given in Eq. (2.44) [110]. In the presence of the fluid flow, we solved the dynamic equations (6.3)–(6.5) numerically. As an initial condition, the variables were set according to the analytical solution of the active straight motion without fluid flow [110], and the active deformable particle was placed at various distances r_{init} from the vortex center. We chose the same system parameters as mentioned in the caption of Fig. 6.2, except that we considered both cases of $a_1 = b_1 = \mp 1$. As mentioned above, in the absence of the fluid flow, the deformation axis tends to be perpendicular to the propulsion direction for $a_1 = b_1 = -1$, whereas it takes a parallel configuration for $a_1 = b_1 = +1$ [110].

On the one hand, for the perpendicular case ($a_1 = b_1 = -1$), we find a steady-state *active circular motion* when $\kappa_1^c < \kappa_1 < 0$, where $\kappa_1^c = -0.5$ for the present parameters. It is the analog of the passive circular motion of $\kappa_1 > 0$. However, in contrast to the passive case, we now obtain only one stable diameter r_0 for each value of $\kappa_1^c < \kappa_1 < 0$. This is indicated by the diamond symbols in Fig. 6.2. Depending on the initial conditions, the active deformable particle either asymptotically approaches this orbit, or it manages to escape from the swirl to infinite distance.

For $\kappa_1 < \kappa_1^c$, the situation becomes markedly different. Starting sufficiently close to the radius r_0 , we still observe the steady-state active circular motion as indicated in

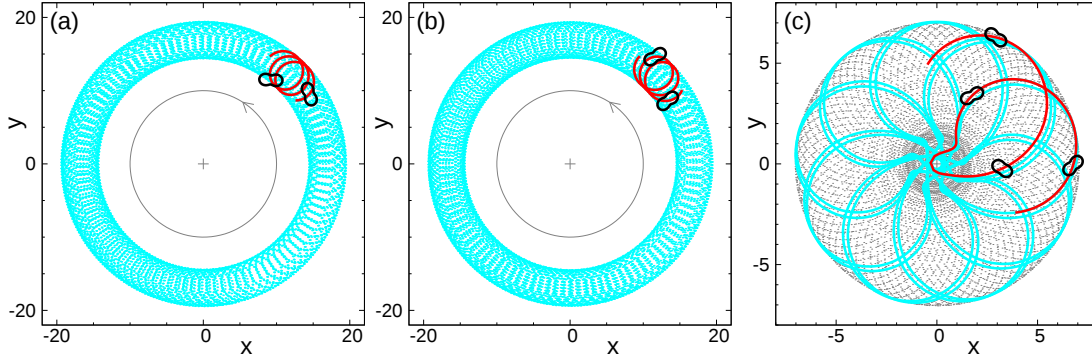


Figure 6.3: Trajectories of (a) and (b) *lunar motions* and (c) a *multi-circular motion*, each for $\kappa_1 = -1$ ($< \kappa_1^c$). Further parameter values are (a) $a_1 = b_1 = -1$ (perpendicular case) and $r_{\text{init}} = 10$, whereas (b) and (c) $a_1 = b_1 = +1$ (parallel case) together with (b) $r_{\text{init}} = 10$ and (c) $r_{\text{init}} = 0.5$. The other parameters are set to $\kappa_2 = 0.5$, $\nu_1 = 1$, and $\mu = 1$. Different colors mark trajectory pieces of different time intervals. Black superimposed silhouettes indicate the shape of the particles.

Fig. 6.2. However, another type of motion occurs depending on the initial conditions. We call it a *lunar-type motion* and depict a typical trajectory in Fig. 6.3(a) for $\kappa_1 = -1$. A short-time piece of the trajectory is emphasised by the thick solid (red) line. The black superimposed silhouettes show the particle orientations and degrees of deformation in an exaggerated way for illustration. We can understand this trajectory as the circular motion that already occurs in the absence of the swirl for $\kappa_1 < \kappa_1^c$ given by Eq. (2.44)² superimposed onto the circular convection due to the vortex flow. In this case, both rotational directions—the one of the smaller revolution, corresponding to the circular trajectory of the moon around the Earth in our heliocentric picture, and the one of the larger revolution, corresponding to the trajectory of the Earth around the sun—have the same sense of rotation as the fluid flow. The radius of the larger revolution depends on the initial condition.

On the other hand, in the parallel case ($a_1 = b_1 = +1$), we did not observe a steady-state active circular motion. Instead, all particles escape far from the vortex center for $0 > \kappa_1 > \kappa_1^c = -0.5$. Therefore designing an active deformable particle in the parallel configuration at low propulsion speed offers a promising strategy to allow escapes. In contrast, for $\kappa_1 < \kappa_1^c$, a particle again undergoes a lunar-type motion. We display a typical trajectory in Fig. 6.3(b). Here, however, the smaller revolution and the fluid flow have opposite sense of rotation, whereas the larger revolution and the fluid flow share the same sense of rotation. This differs from the perpendicular case considered above. Again, the radius of the larger revolution depends on the initial condition.

With decreasing $\kappa_1 \leq -0.7$, the situation gets still more complex in the parallel case. Depending on the initial condition, a *multi-circular motion* can emerge as illustrated in Fig. 6.3(c). The lighter gray, thicker solid (turquoise), and thick solid (red) lines show

² See also Ref. [110].

trajectory pieces of decreasing plot time intervals. To obtain the multi-circular motion, the particle was initially placed relatively close to the vortex center.

In summary, these observations suggest the following escape strategy for an active deformable particle that cannot actively determine its propulsion direction and was dragged into the swirl. If possible, a parallel configuration should be adopted. (Within the framework of Ref. [94] this corresponds to a puller-like propulsion mechanism.) Then the most effective way is not to try too hard to escape; In other words, the effort of self-propulsion should be kept low ($\kappa_1^c < \kappa_1 < 0$). In this combined situation we always observed that the active particle manages to escape.

6.3 Capturing and scattering dynamics

We now study the “collision” of an active deformable particle with the swirl. This is performed in analogy to a classical scattering experiment. Therefore the particle is initially not placed close to the vortex center, but at a comparatively large distance r_{init} away. If the particle was not affected by the flow field of the swirl, it would propel along the direction of its initial velocity orientation. The distance d_{imp} by which it would then miss the vortex center is called the impact parameter. A particle starting from $d_{\text{imp}} = 0$ would hit the center of the vortex, if it were not affected by the swirl flow. The definition of d_{imp} is illustrated in Figs. 6.4(b) and 6.6(b) using example trajectories that we will discuss in more detail below.

If the particle manages to escape from the vortex, we can measure the scattering angle of the event. For this purpose, we determine the angle η_{scat} between the initial velocity orientation and the final velocity orientation when the particle has reached a certain distance r_{esc} from the vortex center.

To keep the setup simple and meaningful in the sense of a scattering experiment, we set the propulsion strength to values $\kappa_1^c < \kappa_1 < 0$. For these values, an active straight motion occurs in the absence of the flow field [110]. We provide this solution as an initial condition at a very large initial distance $r_{\text{init}} = 1.5 \times 10^4$. After numerically integrating Eqs. (6.3)–(6.5) forward in time, we measure the scattering angle at the distance $r_{\text{esc}} = 10^4$ if a scattering event occurs. We varied the values of the propulsion strength κ_1 and the impact parameter d_{imp} , while the other parameters were chosen as before. Due to the swirl geometry, the event of passing the vortex center on one side differs from passing it on the other side. We therefore define $d_{\text{imp}} > 0$ when the particle velocity is initially oriented towards the side of oppositely directed fluid flow. On the contrary, we set $d_{\text{imp}} < 0$ when the particle initially propels towards the side of identically directed fluid flow. See Figs. 6.4(b) and 6.6(b) for illustrations of the definition of the sign of d_{imp} .

We systematically initialised and analysed scattering events as a function of varying impact parameter d_{imp} . Our results are presented in the following, with example trajectories displayed in Figs. 6.4 and 6.6. As can be inferred from the different axes scales of Figs. 6.4 and 6.6, the trajectory parts shown in Figs. 6.4(c) and 6.4(d) and Figs. 6.6(c) and 6.6(d) represent a zoom onto the close vicinity around the swirl center. In this

area, the trajectories have already been significantly bent and influenced by the swirl flow, which becomes obvious from the comparison to Figs. 6.4(b) and 6.6(b). Again, we distinguish between a perpendicular configuration ($a_1 = b_1 = -1$) and a parallel configuration ($a_1 = b_1 = +1$).

6.3.1 Perpendicular configuration

For the perpendicular configuration ($a_1 = b_1 = -1$), the active deformable particle tends to orient its deformation axis perpendicularly to the propulsion velocity. As we saw in the previous section, this is not the best strategy to escape from the vortex. Indeed, as we will see shortly, in a finite interval of impact parameters, the particle gets captured by the swirl instead of being scattered. We discuss the situation as a function of increasing impact parameter.

Generally, the vortex makes the particle deviate from its straight trajectory of motion; See Fig. 6.4(b). For negative impact parameters d_{imp} (not displayed), the particle trajectory is only weakly deformed and the particle leaves the vortex geometry with basically the same velocity orientation as that it had when entering the setup. Thus the scattering angle η_{scat} vanishes. This is true even for weakly positive impact parameters. We recall at this point that the magnitude of the impact parameter and its sign are defined for a quiescent reference situation, measuring by how much and on which side the particle would miss the center in the absence of the swirl flow, respectively. In the presence of the vortex flow, however, the swirl can guide the particle around the vortex center even on the side opposite to the one that the particle is initially heading towards. Still, the net scattering angle η_{scat} can be relatively small in this case. Such a situation is illustrated in Figs. 6.4(a), 6.4(b), and 6.4(c) for $\kappa_1 = -0.3$ and $d_{\text{imp}} = 60$. The scattering angle appears higher in Fig. 6.4(b) due to the rescaled y dimension; See Fig. 6.4(a) for the absolute value.

Further increasing the impact parameter, the scattering process becomes more persistent. Now the particle reaches closer to the vortex center and its trajectory gets significantly bent. This results in a nonzero scattering angle η_{scat} ; See Fig. 6.4(a) and the trajectories for $d_{\text{imp}} = 70$ and 85 in Fig. 6.4(c).

Then, as a function of increasing impact parameter, the active deformable particle more and more gets caught by the swirl. It can happen that the particle circles around the vortex center before it can finally escape from the swirl as depicted by the trajectory for $d_{\text{imp}} = 89$ in Fig. 6.4(c). These events correspond to reorientation processes that are more extreme than simple backscattering, and we indicate them by scattering angles $\eta_{\text{scat}} > \pi$ in Fig. 6.4(a). The scattering angle seems to diverge when the impact parameter is further increased.

At still higher impact parameters, the particle eventually gets captured by the vortex. It cannot escape from the swirl any more. Example trajectories are depicted in Fig. 6.4(d) for $d_{\text{imp}} = 90, 100$, and 103. Interestingly, in all these cases the active deformable particles end up on the same circular trajectory around the vortex center. This attractant type of motion corresponds to the active circular motion discussed in Section 6.2.2.

Finally, when the impact parameter is too large, the particle does not get close enough

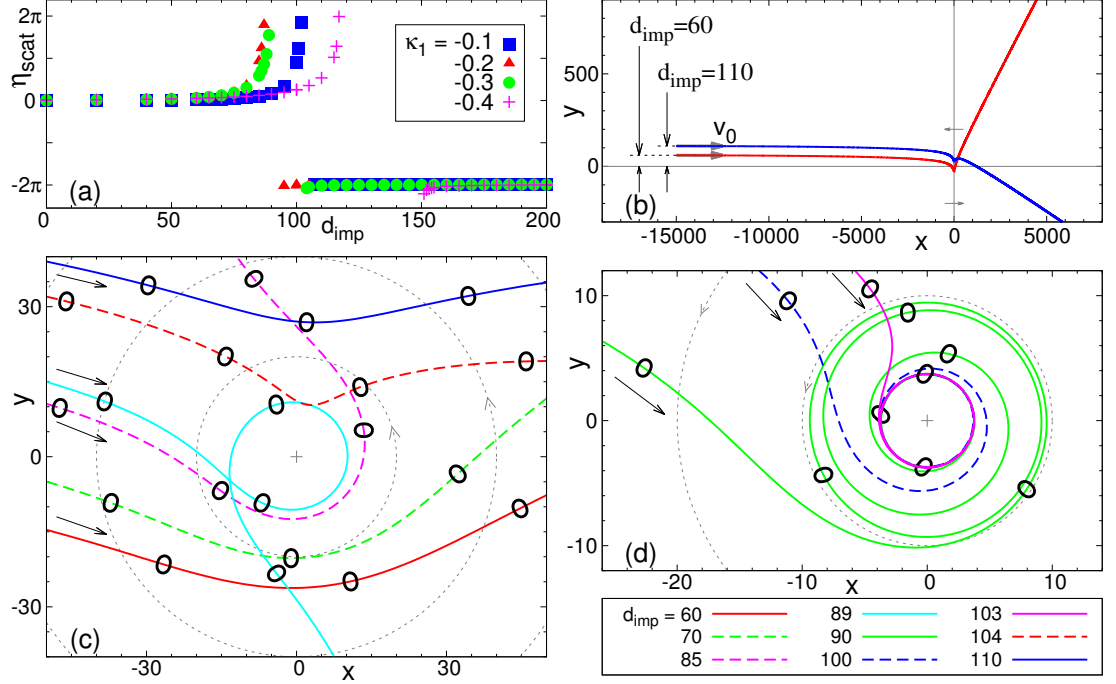


Figure 6.4: Scattering dynamics for $a_1 = b_1 = -1$ (perpendicular case): (a) Scattering angle η_{scat} as a function of the impact parameter d_{imp} for various propulsion strengths κ_1 ; (b) Definition of the impact parameter d_{imp} depicted using example trajectories of incident particles for $\kappa_1 = -0.3$; (c) and (d) Example trajectories for $\kappa_1 = -0.3$ and for different impact parameters d_{imp} . As in the panel (b), the impact parameter d_{imp} measures the distance by which the particle would miss the swirl center if its trajectory were not affected by the swirl flow. The sign of d_{imp} is defined as positive when the particle initially heads towards the side $y > 0$ of oppositely directed fluid flow, whereas it is chosen negative when the particle initially heads towards the side $y < 0$ of identically oriented fluid flow. The gray arrows on the axis $x = 0$ indicate the direction of the swirl flow, pointing to the left for $y > 0$ and to the right for $y < 0$. For illustration, the scales of the x and y axes in the panel (b) are chosen differently and distances in the y direction are enlarged by a factor of ten. In the panels (c) and (d), the black superimposed silhouettes indicate the particle orientations and degrees of deformation and the black arrows mark the direction of motion. Furthermore, the gray dotted lines illustrate the direction of the fluid flow, the vortex center marked by the plus symbol. The panel (c) indicates that there is a finite interval of impact parameters for which the particle cannot escape from the vortex any more but gets captured by the swirl. (Other parameter values are $\kappa_2 = 0.5$, $\nu_1 = 1$, and $\mu = 1$.)

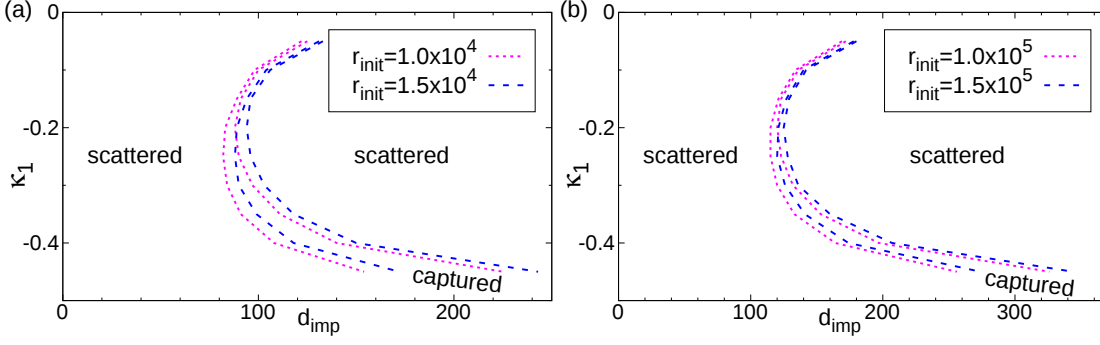


Figure 6.5: Dynamical phase diagram as a function of the impact parameter d_{imp} and the strength of active propulsion κ_1 for the perpendicular case ($a_1 = b_1 = -1$). Two dynamical events are distinguished. Getting scattered by the swirl with a subsequent escape (area outside the lines), and getting captured by the vortex (area between the lines). Our results do not qualitatively depend on the initial distance of the active deformable particle from the vortex center as can be seen when comparing panels (a) and (b) with each other, or when comparing the solid lines with the dashed lines within each panel. Reentrance of the dynamic events can be observed in both directions of the parameter space.

any more to the swirl center to be effectively captured. It now gets scattered again, passing the vortex center on the other side, however. To identify these events of passing on the other side of the swirl in Fig. 6.4(a), we shifted the corresponding scattering angles η_{scat} by -2π . Such events are illustrated in Fig. 6.4(c) by the trajectories for $d_{\text{imp}} = 104$ and 110. The complete trajectory of the scattering event for $d_{\text{imp}} = 110$ is depicted in Fig. 6.4(b).

In effect, we found that the active deformable particle gets scattered by the swirl and can escape for low-enough impact parameters d_{imp} . It gets captured by the swirl at intermediate impact parameters. For large-enough impact parameters, it gets scattered again and can escape. Thus the dynamical behavior of getting scattered is *reentrant* as a function of the impact parameter d_{imp} . Guided by this observation, we scanned the particle behavior in the parameter plane of the impact parameter d_{imp} and the active propulsion strength κ_1 . We distinguished between events of scattering and escape on the one hand and events of capturing on the other hand. The resulting dynamic phase diagram is shown in Fig. 6.5. Most interestingly, the phase behavior is not only reentrant as a function of the impact parameter d_{imp} for fixed propulsion strength κ_1 . Rather, at fixed intermediate impact parameter d_{imp} , we also observe reentrance of the capturing event and a twofold reentrance of the scattering behavior with increasing propulsion strength, i.e., decreasing κ_1 . We checked that our results only slightly vary with the initial distance r_{init} from the vortex center due to the spatial decay of the flow field. Qualitatively our results do not depend on the initial distance r_{init} .

6.3.2 Parallel configuration

For the parallel configuration ($a_1 = b_1 = +1$), the active deformable particle tends to orient its deformation axis along the direction of self-propulsion. This is a good strategy to avoid getting captured by the swirl. Indeed we never observed any event of permanent capturing for such particles that started far from the vortex center with propulsion strengths $\kappa_1^c < \kappa_1 < 0$. Again, we discuss the changes in the dynamic behavior with increasing impact parameter.

While they are heading towards the vortex, the situation for active deformable particles of parallel configuration is just the other way around as for those of perpendicular configuration.³ Their trajectory gets curved into the opposite direction during this initial process; See Fig. 6.6(b). Therefore significant scattering now already takes place for negative impact parameters d_{imp} as demonstrated in Fig. 6.6.

First, for very negative impact parameters d_{imp} , the centre-of-mass trajectory is only slightly influenced by the swirl. The particle passes the vortex with only little net change in the propulsion direction, i.e., η_{scat} is relatively small, as displayed in Figs. 6.6(a), 6.6(b), and 6.6(c) for $\kappa_1 = -0.3$ and $d_{\text{imp}} = -75$. Again, the scattering angle appears higher in Fig. 6.6(b) due to the rescaled y dimension; See Fig. 6.6(a) for the absolute value. Increasing the impact parameter, the particle comes closer to the vortex center and the scattering angle η_{scat} increases; See the trajectory for $d_{\text{imp}} = -71$ in Fig. 6.6(b).

Interestingly, we observe a discontinuous jump of the scattering angle to values $\eta_{\text{scat}} > 2\pi$ in Fig. 6.6(a) at higher impact parameters. The trajectory for $d_{\text{imp}} = -70$ in Fig. 6.6(d) shows the drastic event that occurs in this case and explains the jump in the scattering angle. The particle gets transiently caught by the swirl. Its trajectory describes a loop of more than a full rotation around the vortex center, before the particle can escape with a net scattering angle $\eta_{\text{scat}} > 2\pi$. As indicated by the trajectory for $d_{\text{imp}} = -65$ in Fig. 6.6(d), this behavior persists for further increasing impact parameters. However, the net scattering angle in Fig. 6.6(a) decreases and the loop around the vortex center does not describe a complete rotation of 2π any more.

Remarkably, despite the continuous decrease in the net scattering angles in Fig. 6.6(a), a qualitative difference appears in the trajectories for higher impact parameters. As illustrated for $d_{\text{imp}} = -45$ and -36 in Fig. 6.6(d), the active deformable particle now first passes the vortex center on the opposite side. Still, however, the particle is transiently caught by the swirl and describes a loop around the vortex center as shown in Fig. 6.6(d). As highlighted by the inset of Fig. 6.6(d), the particle in all these cases always performs the loop around the center with the same rotational sense as the fluid flow. This is true independently of the side on which the particle first passes the vortex center. Consequently, in the latter two cases of $d_{\text{imp}} = -45$ and -36 , the particle must switch the side that it exposes to the center of the swirl.

Finally, there is another discontinuous jump of the scattering angle in Fig. 6.6(a) at still higher impact parameters. Corresponding trajectories in Fig. 6.6(c) for $d_{\text{imp}} = -35$ and -25 reveal the reason for this jump. The active deformable particle does not perform

³ Therefore it even looks that the particle that tends to elongate in the parallel direction with respect to the active velocity propels against the swirl flow.

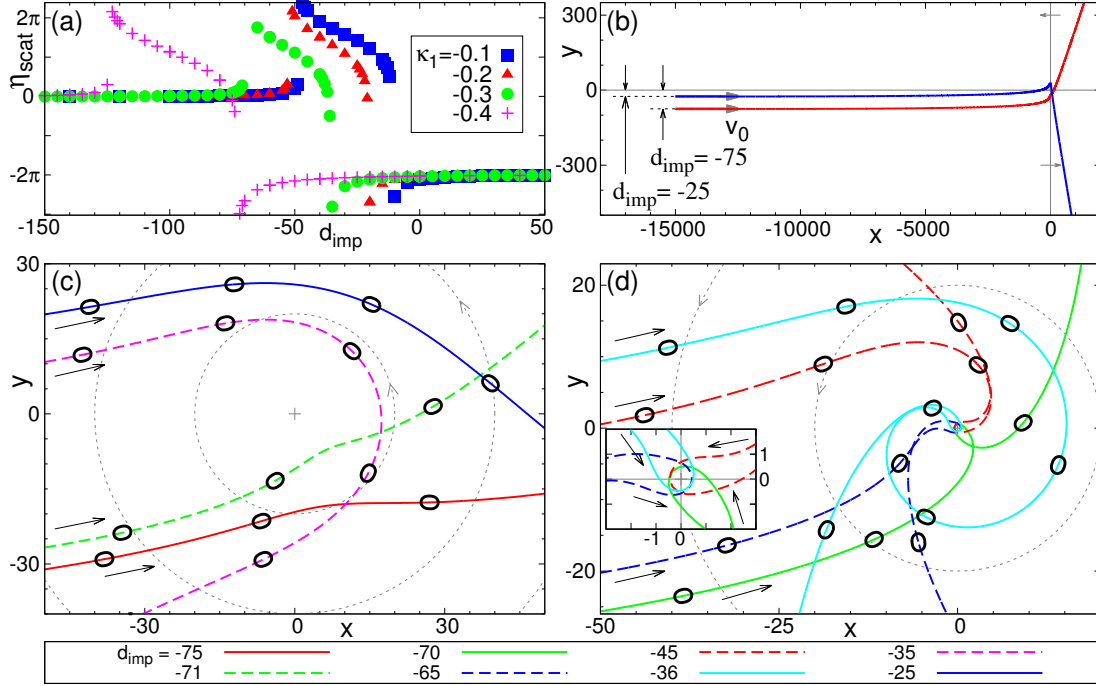


Figure 6.6: Scattering dynamics for $a_1 = b_1 = +1$ (parallel case): (a) Scattering angle η_{scat} as a function of the impact parameter d_{imp} for various propulsion strengths κ_1 ; (b) Definition of the impact parameter d_{imp} depicted using example trajectories of incident particles for $\kappa_1 = -0.3$; (c) and (d) Example trajectories for $\kappa_1 = -0.3$ and for different impact parameters d_{imp} . As in the panel (b), the impact parameter d_{imp} measures the distance by which the particle would miss the swirl center if its trajectory were not affected by the swirl flow. The sign of d_{imp} is defined as positive when the particle initially heads towards the side $y > 0$ of oppositely directed fluid flow, whereas it is chosen negative when the particle initially heads towards the side $y < 0$ of identically oriented fluid flow. The gray arrows on the axis $x = 0$ indicate the direction of the swirl flow, pointing to the left for $y > 0$ and to the right for $y < 0$. For illustration, the scales of the x and y axes are chosen differently and distances in the y direction are enlarged by a factor of ten. In the panels (c) and (d), the black superimposed silhouettes indicate the particle orientations and degrees of deformation and the black arrows mark the direction of motion. In addition, the gray dotted lines illustrate the direction of the fluid flow. No capturing events are observed in this case, but the orbit can come very close to the vortex center. The panel (c) indicates that in a finite interval of intermediate impact parameters, the particle gets transiently caught and loops around the vortex center. As highlighted in the inset, these looping trajectories in close vicinity to the vortex center always show an identical sense of curvature prescribed by the rotational sense of the swirl flow. (Other parameter values are $\kappa_2 = 0.5$, $\nu_1 = 1$, and $\mu = 1$.)

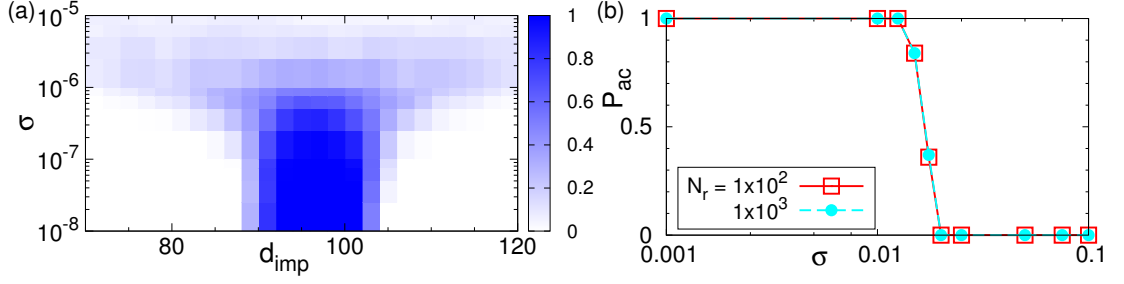


Figure 6.7: Effect of thermal noise on the scattering dynamics. We test the stability of the capturing event for an active deformable particle in the perpendicular configuration that is characterised by the same parameter values as in Fig. 6.4 ($\kappa_1 = -0.3$). (a) Probability for the particle to get captured by the swirl when heading from an initial distance $r_{\text{init}} = 1.5 \times 10^4$ towards the vortex center. The probability is plotted as a function of the impact parameter d_{imp} and the strength σ of the thermal noise. For the color code see the scale bar on the right. (b) Probability P_{ac} of a captured particle to still remain on a captured active circular trajectory after N_r circulations, plotted as a function of the stochastic noise strength σ .

a narrow loop around the vortex center any more. Instead its trajectory features a simple bend around the swirl. We observe events from close to backscattering up to practically no net scattering at all for large impact parameters. Again, for clarity, we shift the scattering angles corresponding to these events by -2π in Fig. 6.6(a). The complete trajectory of the scattering event for $d_{\text{imp}} = -25$ is depicted in Fig. 6.6(b).

6.3.3 Effect of thermal noise

Finally, we ask the question whether thermal noise [91, 140, 144, 175] can qualitatively modify the above results on the scattering and capturing dynamics. In particular, we test the stability of the capturing event against noise and analyse whether the trajectories of the captured state are stable against thermal fluctuations. For this purpose, we add a stochastic force term ξ to the dynamic equation of relative velocity, Eq. (6.4). To keep our argument simple, we consider Gaussian white noise characterised by $\langle \xi_i(t) \rangle = 0$ and $\langle \xi_i(t) \xi_j(0) \rangle = \sigma^2 \delta_{ij} \delta(t)$. Here σ quantifies the strength of the stochastic fluctuations.

Under these conditions we now repeat the scattering experiment that led to the captured states for the perpendicular configuration. The parameters are set to the same values as before (see the caption of Fig. 6.4, $\kappa_1 = -0.3$). We start from the same large initial distance $r_{\text{init}} = 1.5 \times 10^4$ from the vortex center. However, besides the impact parameter d_{imp} , we now vary the noise intensity σ .

Due to the influence of the stochastic force, we now have to measure the probability for the active deformable particle to get captured. For each impact parameter d_{imp} and noise intensity σ , we thus counted the number of capturing and scattering events for repeated runs with different realisations of the stochastic noise. The probabilities were determined from the overall statistics and are shown in Fig. 6.7(a).

At weak noise intensities $\sigma \approx 10^{-8}$, the stochastic effects are negligible and capturing

events occur approximately in the same way as in the deterministic case. To interpret the noise strengths, we use Stokes' relation and Einstein's relation, and we further assume that the thermal noise for active deformable particles is of the same magnitude as in the passive case. We then can attribute the thermal noise of strength $\sigma \approx 10^{-8}$ to a spherical self-propelled droplet of a few millimeters in size in an aqueous solution. At noise intensities $\sigma \approx 10^{-7}$, corresponding to a particle size around one millimeter, the capturing event is still well defined as a function of the impact parameter d_{imp} . In contrast to that, at noise strength $\sigma \gtrsim 10^{-6}$, the stochastic fluctuations smear out the statistics and a capturing event is not well defined any more. The intensities of thermal noise about $\sigma \approx 10^{-6}$ and $\sigma \approx 10^{-5}$ identify spherical objects of a few hundred and one hundred micrometers in size, which come into the range of large microorganisms.

The reason for the fading of the capturing event in the latter case is not related to the captured states becoming unstable, however. This can be seen by considering captured particles on their active circular motion around the vortex center and exposing them to the stochastic force. We measured the probability P_{ac} of finding the particles still captured after a certain number N_r of circulations around the swirl. In practice, we checked whether they are still within a certain threshold distance from the vortex center. Our results are summarised in Fig. 6.7(b).

It is obvious that the active deformable particles can escape from the captured states only at much higher noise intensities than the ones referred to in Fig. 6.7(a). The fading probabilities of getting captured at higher noise strengths σ in Fig. 6.7(a) therefore do not imply that the captured states become unstable. Rather, due to the noise, the particles increasingly depart from their deterministic trajectories towards the swirl center and do not hit the vortex any more. This can easily be cured if the incident particles are placed closer to the vortex center in a modified initial condition. Therefore, despite thermal noise, the active deformable particles should show the predicted dynamics.

6.4 Summary and conclusions

In summary, we studied the dynamic behavior of an active deformable particle in a swirl flow. To our knowledge this geometry has not been investigated before for active particles, although it is a setup of high practical relevance and straightforward to be realised in an experiment. Within our framework, we distinguished between two types of particles: those that tend to elongate perpendicularly to their propulsion direction and those that prefer a parallel configuration. Considering droplets propelling due to chemical reactions, a recent theoretical study suggests that the first ones can be classified as pushers, while the second ones are pullers [94].

For the different types of deformable particles, we found different bound states in the swirl. Passive deformable particles show *passive circular motion*, where not all radii are stable depending on the friction with the fluid environment. Active deformable particles at lower strength of self-propulsion and in the perpendicular configuration either escape from the swirl, or they feature an *active circular motion* of one stable radius determined by their activity. In the parallel configuration they always escape from the swirl. Beyond

a threshold for the strength of self-propulsion, the particles could not escape any more but showed an *active circular motion*, a *lunar-type motion*, or a *multi-circular motion*, depending on the particle configuration and on the initial conditions.

Second, in analogy to classical scattering experiments, we investigated how active deformable particles interact with the swirl when they are heading towards the vortex from far away in a straight motion. For active particles of perpendicular configuration we observed that they were *captured* by the swirl on a trajectory of the active circular motion at intermediate impact parameters. This capturing event is *reentrant* as a function of the strength of self-propulsion. For other impact parameters the particle is *scattered* and manages to escape. The scattering event is *reentrant* as a function of the impact parameter and *twofold reentrant* as a function of the strength of self-propulsion. In contrast to that, we observed that active particles in the parallel configuration are *always scattered*. Thus, to design an active deformable particle that is not captured by swirls, the parallel configuration should be preferred and the strength of self-propulsion should be weak enough to avoid a circular motion. Nevertheless, scattered particles may perform interim loops around the vortex center at very close distances, possibly changing the side that they expose to the vortex center. Additional thermal noise was not found to qualitatively alter the capturing dynamics in an appropriately chosen setup.

The swirl flow geometry is of high practical relevance and straightforward to be realised in an experiment. In principle, a magnetic stir bar on the bottom of a water tank is enough to create the vortex flow. Self-driven droplets on the water surface constitute appropriate deformable active particles [38, 40] that propel in a quasi-two-dimensional environment. Therefore they should immediately allow us to test and verify our predictions in an actual experimental setup. This system should be easier to realise than the typically investigated flow profiles of linear shear. Apart from that, also on the theoretical side several questions directly follow from our study. Most notably, it will be worthwhile also to analyse the particle behavior in flow fields of non-vanishing local vorticity or even in turbulent flows. On the one hand, hydrodynamically enforced trapping and particle segregation can occur for passive particles in a vorticity flow [176, 177]. On the other hand, microswimmers were observed to create turbulence-like flows even by themselves in dense suspensions [156, 178, 179]. Apart from that, it has been reported that active particles not only self-propel but also actively rotate [40, 108, 111–113, 129, 144, 145, 180–189]. It will be very interesting to see how the active rotation interact with the rotational component of the flow fields and what their impact is on the dynamics. We thus hope that our results will stimulate further investigations both on the theoretical and the experimental side to elucidate the dynamics of active particles in external flow fields.

6.A Stability analysis

In this Appendix, we describe the details of the stability analysis of the steady-state solutions of Eqs. (6.3)–(6.5). First, for the vortex flow specified by Eq. (6.1), the strain rate tensor of the flow field follows via Eq. (6.2). At the particle position $\mathbf{x}$, parameterized by Eq. (6.6), we obtain

$$\mathbf{A} = \begin{pmatrix} \mu r^{-2} \sin 2\eta & -\mu r^{-2} \cos 2\eta \\ -\mu r^{-2} \cos 2\eta & -\mu r^{-2} \sin 2\eta \end{pmatrix}. \quad (6.14)$$

Inserting it together with the parameterization Eqs. (6.6)–(6.8) into Eqs. (6.3)–(6.5), the equations of motion can be rewritten in the form

$$\frac{dr}{dt} = v \cos(\Theta - \psi), \quad (6.15)$$

$$\frac{dv}{dt} = -\kappa_1 v - v^3 - a_1 v s \cos 2\psi, \quad (6.16)$$

$$\frac{ds}{dt} = -\kappa_2 s + \frac{b_1}{2} v^2 \cos 2\psi - \nu_1 \mu r^{-2} \sin 2\Theta, \quad (6.17)$$

$$\frac{d\Theta}{dt} = -\frac{b_1}{4s} v^2 \sin 2\psi - v r^{-1} \sin(\Theta - \psi) - \mu r^{-2} \left(1 + \frac{\nu_1}{2s} \cos 2\Theta\right), \quad (6.18)$$

$$\frac{d\psi}{dt} = \left(a_1 s - \frac{b_1}{4s} v^2\right) \sin 2\psi - \frac{\nu_1}{2s} \mu r^{-2} \cos 2\Theta. \quad (6.19)$$

We have here defined $\Theta = \theta_2 - \eta$ and $\psi = \theta_2 - \phi$.

Following the general procedure, we investigate the stability of the steady-state solutions of these equations via the eigenvalues of the corresponding linear stability matrix. Its components are defined by

$$\mathcal{L}_{ij} = \frac{\partial}{\partial \mathcal{X}_j} \left(\frac{d\mathcal{X}_i}{dt} \right), \quad (6.20)$$

where $\mathcal{X} = (r, v, s, \Theta, \psi)$. We obtain the eigenvalues λ of $\mathcal{L}$ as usual from the condition

$$\det(\mathcal{L} - \lambda \mathcal{I}) = 0, \quad (6.21)$$

with $\mathcal{I}$ the unity matrix. The corresponding motion is stable, if all $\lambda < 0$; Marginally stable, if all $\lambda \leq 0$, while it becomes unstable, if at least one $\lambda > 0$.

From Eq. (6.16), two types of steady-state solutions follow. One of them describes a passive motion of $v = 0$, i.e. the particle is simply advected by the fluid flow. The other one corresponds to an active translational motion given by the relative speed $v = \sqrt{\Gamma}$ with respect to the surrounding fluid, where

$$\Gamma = -\kappa_1 - a_1 s \cos 2\psi. \quad (6.22)$$

In the remaining part of this Appendix, we carry out the linear stability analysis of the passive motion.

6 Active deformable particle in a swirl

For the passive motion $v = 0$, Eq. (6.15) implies that the distance r from the vortex center remains constant. We thus obtain circular trajectories of fixed radius $r = r_0$ in the passive case. This is why we term this kind of motion the *passive circular motion*. The complete steady-state solution is found by setting the remaining time derivatives in the above dynamic equations equal to zero. Taking into account that $v = 0$, it then follows from Eq. (6.17) that

$$s = -\frac{\nu_1}{\kappa_2} \mu r_0^{-2} \sin 2\Theta. \quad (6.23)$$

Likewise, from Eq. (6.18) together with Eq. (6.17), we obtain

$$\tan 2\Theta = \frac{\kappa_2 r_0^2}{2\mu}. \quad (6.24)$$

The dynamic equation Eq. (6.19) can be ignored at this point because it determines the relative orientation of the relative velocity $\mathbf{v}$, which vanishes in the case of passive circular motion $v = 0$. Naturally, it becomes important in the following when we study the bifurcation from the passive circular motion ($v = 0$) to other types of motion characterised by $v \neq 0$.

We determined the eigenvalues of the linear stability matrix for the passive circular motion via Eq. (6.21). They are obtained as $\lambda_r = 0$, $\lambda_v = \Gamma$, $\lambda_\psi = 2a_1 s \cos 2\psi$, and as the eigenvalues $\lambda_\pm$ of the submatrix

$$\mathcal{L}^{\text{sub}} = \begin{pmatrix} -\kappa_2 & -2\nu_1 \mu r_0^{-2} \cos 2\Theta \\ \frac{1}{2} \nu_1 \mu r_0^{-2} s^{-2} \cos 2\Theta & \nu_1 \mu r_0^{-2} s^{-1} \sin 2\Theta \end{pmatrix}. \quad (6.25)$$

On the one hand, since $s > 0$ (being the magnitude of deformation), we conclude from Eq. (6.23) that $\nu_1 \mu \sin 2\Theta < 0$. Consequently, $\text{tr } \mathcal{L}^{\text{sub}} < 0$ and $\det \mathcal{L}^{\text{sub}} > 0$. This leads to $\lambda_\pm < 0$, which is necessary for stability. On the other hand, the eigenvalue $\lambda_r = 0$ implies that the stability is at most marginal. However, we still need to consider the signs of the eigenvalues λ_v and λ_ψ . Both λ_v and λ_ψ depend on ψ , so we now take into account Eq. (6.19).

In the case of the passive circular motion, the steady-state solution of Eq. (6.19) follows as

$$\sin 2\psi = \frac{\kappa_2}{a_1 \nu_1 \sin 2\Theta}. \quad (6.26)$$

This expression does not determine the sign of $\cos 2\psi$. Thus there is always a solution that guarantees the condition $\lambda_\psi = 2a_1 s \cos 2\psi \leq 0$ necessary for marginal stability. Nevertheless, we must satisfy $\sin^2 2\psi \leq 1$ for the steady-state solution to exist. This leads to the condition $r_0 \geq r_{0,\min}$ with $r_{0,\min}$ given by

$$r_{0,\min} = (2|\mu|)^{1/2} \left\{ (a_1 \nu_1)^2 - \kappa_2^2 \right\}^{-1/4}. \quad (6.27)$$

Taking into account Eqs. (6.22) and (6.23) together with the last eigenvalue $\lambda_v = \Gamma$, we need to require

$$\lambda_v = \Gamma = -\kappa_1 + a_1 \cos 2\psi \frac{\nu_1 \mu r_0^{-2}}{\kappa_2} \sin 2\Theta < 0 \quad (6.28)$$

for the solution $v = 0$ to be stable. Together with Eqs. (6.26) and (6.24), we obtain $\kappa_1 > \kappa_1^\dagger$ with $\kappa_1^\dagger$ given by

$$\kappa_1^\dagger = \frac{2\mu^2}{r_0^2 r_{0,\min}^2} \left(\frac{r_0^4 - r_{0,\min}^4}{\kappa_2^2 r_0^4 + 4\mu^2} \right)^{1/2} > 0. \quad (6.29)$$

When r_0 approaches $r_{0,\min}$ from above, we find that $\kappa_1^\dagger$ tends to zero.

Finally, when $r_0 < r_{0,\min}$, the steady-state solution for ψ does not exist. Equation (6.19) then implies that ψ monotonically increases or decreases, depending on the parameters. Then, on average, $\cos 2\psi$ vanishes, and Eq. (6.28) reduces to $\kappa_1 > 0$ for $r_0 < r_{0,\min}$. We tested and confirmed this observation numerically (see also Fig. 6.2). Our results are summarised by the necessary condition in Eq. (6.11) for the passive circular motion to be marginally stable.

Equations (6.27), (6.29), and (6.11) imply that for an increasing stiffness of the particle (i.e., increasing κ_2) the stability range of the passive circular steady-state solution increases. This can be seen as follows. As κ_2 approaches $|a_1 \nu_1|$ from below, the value of $r_{0,\min}$ diverges. For $\kappa_2 \geq |a_1 \nu_1|$, the condition for κ_1 in Eq. (6.11) extends to the full range of $\kappa_1 > 0$. This corresponds to the natural requirement that the passive particle suffers from the friction with its fluid environment, with $\kappa_1 > 0$ setting the friction parameter. Thus, in this case, circular steady-state trajectories of all radii are marginally stable.

Chapter 7

Summary and conclusions

To summarise this thesis, we investigated the dynamics of active deformable particles theoretically. Considering the existence of an external flow field, we introduced variables to describe an active deformable particle. First of all, the external flow is measured by the flow velocity $\mathbf{u}$, which is a function of space. As usual, the spacial derivative of the flow velocity is separated into two contributions: namely, the elongational and rotational contributions, which correspond to the symmetric tensor $\mathbf{A}$ and the antisymmetric tensor $\mathbf{W}$, respectively. The centre-of-mass velocity of the particle in a flow field then divided into the flow velocity $\mathbf{u}$ representing the advection due to the external flow and its relative velocity $\mathbf{v}$. The relative velocity, or the deviation of the velocity from the surrounding flow velocity, originates from the spontaneous translational motion of the particle. Therefore we named it as an active velocity in this thesis. In the same manner, the rotation of the particle is described as a summation of the rotation due to the surrounding flow and its relative rotation. Since the rotational contribution of the flow is represented by the antisymmetric tensor $\mathbf{W}$, it is natural to describe the relative rotation by an antisymmetric tensor variable $\mathbf{\Omega}$ as well. We referred to it as active rotation since the relative rotation results from the spontaneous rotational motion of the particle. Finally, the deformation of the particle is described by symmetric tensor variables, which we named symmetric deformation tensors. The symmetric deformation tensor of order n corresponds in a two dimensional space to the n th-order Fourier mode of the shape deformation. As a result, we introduced the vector and tensor expressions of the centre-of-mass position and velocity given by the vector variables, the rotation of the particle represented by the antisymmetric tensor, and the deformation of the particle shape described by the symmetric tensors. For these variables, we derived time-evolution equations from symmetry arguments. In particular we concentrated ourselves on the following two topics.

First, we propound the argument that there are at least two types of spinning motion for active deformable particles. On the one hand, an active particle undergoes a spinning motion as a whole body, which we called a type-I spinning motion in this thesis. For this type-I spinning motion, the active rotation is defined, which is related to an active angular velocity. On the other hand, when the particle is soft and hence does change its shape, the deformation of the particle shape may travel along the interface. In terms

7 Summary and conclusions

of the dynamics of the particle, this traveling wave of shape deformation is regarded as a spinning motion. We referred to this spinning motion as a type-II spinning motion in this thesis, to distinguish from the type-I spinning motion. Indeed, for this type-II spinning motion the deformability of the particle shape plays an important role, and the particle is not required to rotate as a whole body. In contrast, the type-I spinning motion corresponds to the spinning motion of a rigid body and hence the shape of the particle is not necessarily deformable.

In order to confirm this proposition, we demonstrated the dynamics of active deformable particles in a quiescent flow field, where the effect of the surrounding flow is negligible. In Chapter 3, we introduced a model of an active deformable particle that undergoes the type-I spinning motion. Two basic active motions were taken into account: the active translational motion of the centre of mass represented by the active velocity vector as well as the active rotation around the centre of mass characterised by the antisymmetric tensor variable. For these variables, together with a traceless symmetric second-order tensor variable corresponding to the elliptical deformation, coupled nonlinear equations of motion are derived from symmetry considerations. Besides the spinning motions with and without deformation, both of which correspond to the type-I spinning motion, several dynamical solutions such as circular motions and quasi-periodic motions are obtained.

In contrast, we discussed the model equations to realise the type-II spinning motion in Chapter 4. We considered time-evolution equations of an active deformable particle without the active rotation, but instead we took into account higher order deformations. We first showed a mathematical symmetry of the coupled quadratic equations of the n th and $2n$ th-order deformations for different integer n . Then, as the simplest case to achieve our purpose, we investigated the equations of motion for the quadratic and quartic deformations. We predicted the existence of a spinning motion theoretically and confirmed it numerically as well. Since the variables for the active and passive rotation of the particle are absent, the spinning motion obtained with this model is definitely different from the type-I spinning motion. Indeed, it is a type-II spinning motion, where the deformation of the shape travels along the interface of the particle. In this case, we also found continuous and intermittent oscillations of the shape deformation and an oscillatory-spinning motion.

The second topic of this thesis is the dynamics of active deformable particle in an external flow field. We introduced the contribution of the external flow field to the time-evolution equations of the active deformable particle by using the same strategy as above, i.e. by symmetry considerations. Particularly, two different flow geometries are studied in detail. One is a linear shear flow as one of the simplest flow geometries. For a small shear rate, the active deformable particle undergoes dynamical motions that the particle exhibits in the absence of the external flow in addition to the advection due to the external flow. The resulting motions are active and passive straight motions, a cycloidal motion, and a quasi-periodic motion. Increasing the shear rate, the dynamics became more complicated; Namely a periodic motion, winding motions, regular and undulated cycloidal motions, and even chaotic behaviours were obtained. Interestingly, when the active rotation does not exist and when the active rotation does exist in the

opposite direction to the direction of the rotation due to the flow, the active deformable particle exhibits a straight motion for a finite range of large shear rate. This active straight motion for large shear rate was not observed for the particle with the active rotation in the same direction as the flow rotation. Such a straight motion was observed for an active rigid circular particle as well, but only for the exact value of the shear rate to balance the active rotation. These results are summarised in Chapter 5.

Besides the linear shear flow, we considered the dynamics of active deformable particles in a swirl, which is discussed in Chapter 6. As far as we know, there has been no study concerning of motion of active particles in a swirl except ours, although swirl flows naturally occur in many situations. We investigated steady-state solutions of the equations of motion, and found different dynamical motions. Passive deformable particles show a passive circular motion, where it is simply advected by the flow on circles around the vortex centre with its shape elongated. We found that there is prohibited intermediate distance from the swirl centre when the particle deformability is larger than a threshold value, unlike passive rigid circular-shaped particles. In contrast, active deformable particles with the tendency to elongate perpendicularly with respect to the active velocity either escape from the swirl or undergo an active circular motion, where one specific value of radius is stably determined depending on the strength of their activeness when the self-propulsion strength is low. When the strength of self-propulsion is beyond a threshold, the active particles are unable to escape any more but exhibit either the active circular motion or a lunar-type motion. On the other hand, active deformable particles that tend to elongate parallel to the active velocity always escape from the swirl below the threshold, whereas for larger active propulsion they exhibit a lunar-type motion or a multi-circular motion, depending on the initial condition. In addition to the analysis of steady-state solutions, we carried out numerical experiments in an analogous setup to classical scattering experiments in the context of active matter, by preparing active deformable particles heading towards the vortex centre. When the particle has a tendency to elongate parallel to the active velocity, the active deformable particle is always scattered by the swirl. Contrary, when they tend to be perpendicular, then the active deformable particles are not only scattered but also captured by the swirl flow depending on how close they can get to the vortex centre. These results suggest the following escape strategy for an active deformable particle that cannot actively determine its propulsion direction and was dragged into the swirl. If possible, a parallel configuration should be adopted. (Within the framework of Ref. [94] this corresponds to a puller-like propulsion mechanism.) Then the most effective way is to keep the strength of active propulsion low and not to try too hard to escape. In this combined situation we always observed that the active particle manages to escape. Otherwise, the particle might get caught by the swirl and be unable to escape, which possibly leads to death for living organisms.

We now mention the derivation of the time-evolution equations from continuous models. The time-evolution equations introduced in this thesis are derived phenomenologically, but some of them have already been derived from detailed models. The set of time-evolution equations (2.29)–(2.31) has been obtained by interfacial method from reaction-diffusion equations [102, 105], where an isolated domain suffers translational

7 Summary and conclusions

instability. In addition to that, it has also been derived in a similar way from partial-differential equations of a liquid droplet in a Stokesian fluid solution [94, 107], where a chemical reaction takes place on the interface. Equations (4.1)–(4.5), in principle, can also be derived in the same procedure. However, the derivation of the equations including the particle rotation still remains as an open question. Furthermore, the derivation of the equations of motion of active deformable particles in an external flow field from fluid-dynamical equations is another interesting problem that is to be clarified.

Our predictions can in principle be verified experimentally. One possible realisation may be active liquid droplets floating on an aqueous phase. An external linear shear flow can be obtained by sliding one pair of the facing walls of the bath container alongside in opposite directions. The swirl is generated more easily for instance by using magnetic stir bars. On the other hand, the two types of spinning motion are already found in experiments. In Ref. [123], Ebata *et al.* found that a liquid droplet floating on another liquid bath, where the whole system is vibrated in the vertical direction, exhibits both type-I and type-II spinning motions, depending on e.g. the vibration frequency. In this case, they measured the flow profile inside the droplet and found that the flow rotates in the same direction as the particle rotation in the case of the type-I spinning motion whereas the flow rotates in the opposite direction for the type-II spinning motion. They showed that their experimental results can be reproduced by using the model equations almost same as Eqs. (4.1)–(4.5).

Future related problems are briefly discussed. One is the derivation of the equations of motion from other detailed models as mentioned above. Besides, quantitative comparison with experiments is required, which should be achieved if the phenomenological equations are derived from detailed continuous models of interest. Finally, although we have developed equations of motion for active deformable particles by taking into account the centre-of-mass position and velocity, the particle rotation, and the shape deformation, these are actually macroscopic variables and the mesoscopic and microscopic internal degrees of freedom are lacking. Therefore models that include such internal structures of the active particle should be developed. Indeed, in biological systems such as living cells, it is known that the macroscopic movement is strongly related to the dynamics of the internal structures.

In conclusion, active matter is a broad new concept. The example of active matter varies from synthetic materials to biological living organisms. Thanks to this comprehensive conception, a physical viewpoint to discuss living and non-living systems on the same stage is provided. Therefore, on the theoretical side of the study of active matter, besides detailed modellings to understand each specific active system, general descriptions to capture universal features are necessary to be developed. In this thesis, we addressed one aspect of this point especially in terms of active deformable particles. Indeed the model equations are derived from symmetry considerations and thus do not depend on any specific mechanism of active motion. Therefore, the series of our works may give one possible way toward such descriptions. It is of great importance to understand basic dynamical motions and clarify their origin by using simple models, which is expected to provide a key route to elucidate complicated dynamics in real systems.

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