A SIMPLE DERIVATION OF ROTNE–PRAGER TENSOR AND HYDRODYNAMIC INTERACTIONS BETWEEN TWO SPHERES*

Qiyi Zhang†, Xun Xiang

Department of Mathematics and Physics
Chongqing University of Science and Technology
Chongqing, 401331, China

(Received June 10, 2011; revised version received November 2, 2011)

We have given a simpler derivation of the Rotne–Prager tensor based on the exact fluid velocity formula for a uniform flow past a sphere in low Reynolds number regime. For two identical spheres in uniform flow, we have given the hydrodynamic interaction profiles for different distances and angles, which are formed between the flow directions and the connection lines of two spheres. The lift forces perpendicular to the flow directions are responsible for the migration phenomenon in the vorticity direction of a chiral object in shear flow.

DOI:10.5506/APhysPolB.43.111
PACS numbers: 47.15.G–, 05.60.Cd, 46.70.Hg

1. Introduction

In the low Reynolds number regime, the fluid flow velocity at an arbitrary point $\boldsymbol{r}$ is linearly related to a point force $\boldsymbol{f}(\boldsymbol{R})$ at $\boldsymbol{R}$ by $u(\boldsymbol{r}) = H(\boldsymbol{r}-\boldsymbol{R})\boldsymbol{f}(\boldsymbol{R})$. The mobility tensor, H, describing the hydrodynamic interactions, can be very complicated, and obtaining analytical expressions is very difficult [1]. As is well known, the exact hydrodynamic interaction tensors of two spheres are essentially not pairwise-additive, they are long-range, and can be expressed as a power series in a/r [2,3,4,5,6,7,8], where a is the sphere radius and r is the distance between centers of the two spheres. However, the mathematical expression for H is greatly simplified if the following assumptions are made: (1) the particles are all spherical; (2) hydrodynamic

* This research is funded by the Chongqing Natural Science Foundation (Grant No. CSTC 2011BB0110) and National Natural Science Foundation of China (Grant No. 20804060).

† qyzhang520@163.com

interaction is pair-wise additive; (3) the distance between two spheres is much larger than the diameter of the sphere $2a$; and (4) no-slip boundary conditions are used on sphere surfaces. Then, H is expressed as functions of the particle positions and velocities, without explicitly dealing with the fluid motions. The Oseen and Rotne–Prager tensors [9] are the lowest order terms in power series of hydrodynamic interactions; the former neglects the size of the particle, while the latter takes into account some corrections to the particle size. The Rotne–Prager tensor is of central importance in various interdisciplinary fields such as microfluidics [10,11] and biophysics [12,13].

The present work is based on the above approximations.

Here, based on the exact flow velocity formula for a sphere in uniform flow under the low Reynolds number limit, we will give a simpler derivation of the Rotne–Prager tensor.

A phenomenon has triggered much interest in recent years, that the lift force (or migration direction) of chiral objects in shear flow can be aligned with either vorticity direction or opposite vorticity direction depending on different handedness [14, 15]. The chiral objects, even many other rigid objects and biological macromolecules, are often theoretically modeled by using a distribution of Stokeslets on the body surface [15,16]. Hence, Rotne–Prager tensor is widely accepted in the description of hydrodynamics of these Stokeslets, where each Stokeslet is considered as point-particle with fixed position and no rotation. Higher order contributions such as many-body [17,18,19], coupling between rotational and translational motions [3], and lubrication forces [20,21] are neglected.

Motivated by this phenomenon and based on the above approximations, we thus carry out researches on an old simple issue related to the hydrodynamics of two identical spheres in uniform flow. Although many studies had been done on this kind of problem [22,23,24,25,26,27], we especially focus on the lift forces perpendicular to the flow directions, for different angles between the flow directions and the connection lines of two spheres, and different distances between two spheres, because it is partially responsible for explanation of migrations in the vorticity direction for chiral objects in shear flow [28].

2. A simple derivation of Rotne–Prager tensor

According to the exact results for the fluid velocity that obeys the creeping flow equation due to the presence of a sphere, we will derive the expressions of Rotne–Prager tensor by transformation of the flow velocity expressions from spherical coordinates to Cartesian coordinates, on the base of the above approximations in Sec. 1 with the particles treated as point-like objects and their rotation effects neglected.

In a creeping uniform flow u_0, a sphere with radius a excites a flow field at distance r from the center of sphere [29, 30]

$$u_r(r,\theta) = u_0 \cos\theta + u_0 \cos\theta \left(\frac{1}{2}\frac{a^3}{r^3} - \frac{3}{2}\frac{a}{r} \right) , \tag{1a}$$

$$u_\theta(r,\theta) = -u_0 \sin\theta + u_0 \sin\theta \left(\frac{1}{4}\frac{a^3}{r^3} + \frac{3}{4}\frac{a}{r} \right) , \tag{1b}$$

where the flow is along the direction of $\theta = 0$ in polar coordinates.

Suppose the flow velocity is of arbitrary direction in Fig. 1, we can decompose $\boldsymbol{u}_0$ into $\boldsymbol{u}_0 = u_{0x}\boldsymbol{i} + u_{0y}\boldsymbol{j} + u_{0z}\boldsymbol{k}$. We take the u_{0y} component as an example, substitute u_{0y} and θ_y into Eq. (1), get the corresponding u_r and u_θ, which are expressed further in xyz coordinates

$$u_x = (u_r \sin\theta_y + u_\theta \cos\theta_y)\cos\alpha\, , \tag{2a}$$

$$u_y = u_r \cos\theta_y - u_\theta \sin\theta_y\, , \tag{2b}$$

$$u_z = (u_r \sin\theta_y + u_\theta \cos\theta_y)\cos\beta\, . \tag{2c}$$

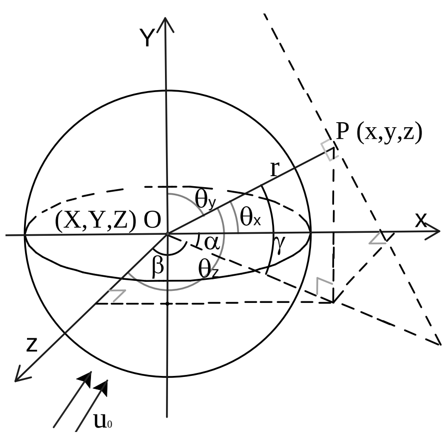

Fig. 1. The schematic of the geometric relation for a sphere with center located at point O(X, Y, Z) in uniform flow u_0. The position P(x, y, z) with distance r away from the sphere center specifies three angles θ_x, θ_y and θ_z, which are formed by the OP connection line and three coordinate axes. γ is angle between the connection line OP and its projection line on xoz plane. α and β are formed by this projection line and two axes on xz plane.

Using the simple relations of triangle functions, $\sin\theta_y \cos\alpha = \cos\gamma\cos\alpha = \cos\theta_x$, $\sin\theta_y\cos\beta = \cos\gamma\cos\beta = \cos\theta_z$, the above flow velocity of Eq. (2) can be transformed to

$$u_x = \frac{3}{4}u_{0y}\left(\frac{a^3}{r^3} - \frac{a}{r}\right)\cos\theta_y\cos\theta_x\,, \tag{3a}$$

$$u_y = u_{0y}\left[1 + \left(\frac{1}{2}\frac{a^3}{r^3} - \frac{3}{2}\frac{a}{r}\right)\right]\cos^2\theta_y + u_{0y}\left[1 - \left(\frac{1}{4}\frac{a^3}{r^3} + \frac{3}{4}\frac{a}{r}\right)\right]\sin^2\theta_y\,, \tag{3b}$$

$$u_z = \frac{3}{4}u_{0y}\left(\frac{a^3}{r^3} - \frac{a}{r}\right)\cos\theta_y\cos\theta_z\,. \tag{3c}$$

For convenience of calculation, all the triangle functions are substituted by $\cos\theta_x = \frac{x-X}{r}, \cos\theta_y = \frac{y-Y}{r}, \cos\theta_z = \frac{z-Z}{r}$

$$u_x = u_{0y}\left[-\frac{3}{4}a\frac{(y-Y)(x-X)}{r^3} + \frac{1}{4}a^3\left(3\frac{(y-Y)(x-X)}{r^5}\right)\right]\,, \tag{4a}$$

$$u_y = u_{0y} + u_{0y}\left[-\frac{3}{4}a\left(\frac{1}{r} + \frac{(y-Y)^2}{r^3}\right) + \frac{1}{4}a^3\left(-\frac{1}{r^3} + 3\frac{(y-Y)^2}{r^5}\right)\right]\,, \tag{4b}$$

$$u_z = u_{0y}\left[-\frac{3}{4}a\frac{(y-Y)(x-X)}{r^3} + \frac{1}{4}a^3\left(3\frac{(y-Y)(x-X)}{r^5}\right)\right]\,. \tag{4c}$$

Considering the contributions from the other two components u_{0x} and u_{0z}, we can use the following Stokeslets tensor (*i.e.*, the Oseen tensor) and Doublets tensor

$$S_{ij}(\boldsymbol{x}, \boldsymbol{R}^\mu) = \frac{\delta_{ij}}{r} + \frac{(x_i - R_i^\mu)\left(x_j - R_j^\mu\right)}{r^3}\,, \tag{5a}$$

$$D_{ij}(\boldsymbol{x}, \boldsymbol{R}^\mu) = -\frac{\delta_{ij}}{r^3} + 3\frac{(x_i - R_i^\mu)\left(x_j - R_j^\mu\right)}{r^5}\,, \tag{5b}$$

where μ is the sphere label, $r = |\boldsymbol{x} - \boldsymbol{R}^\mu|$, i and j run from 1 to 3. So, the flow field can be written as [31]

$$u_i(\boldsymbol{x}) = u_{0i} + \sum_j u_{0j}\left[-\frac{3}{4}aS_{ij}(\boldsymbol{x}, \boldsymbol{R}^\mu) + \frac{1}{4}a^3 D_{ij}(\boldsymbol{x}, \boldsymbol{R}^\mu)\right]\,. \tag{6}$$

If there are many spheres in the fluid, the flow field should be the superposition of the contributions of all the spheres

$$u_i(\boldsymbol{x}) = u_{0i} + \sum_{\mu j}(6\pi\eta a f_{\mu j} u_{0j})\left[-\frac{S_{ij}\left(\boldsymbol{x}, \boldsymbol{R}^\mu\right)}{8\pi\eta} + \frac{a^2 D_{ij}\left(\boldsymbol{x}, \boldsymbol{R}^\mu\right)}{24\pi\eta}\right]\,, \tag{7}$$

where η is the flow viscosity, $f_{\mu j}$ is a coefficient associated with the μ-th sphere contributions to the flow field. Obviously, $F_{\mu j} = 6\pi\eta f_{\mu j} u_{0j} a$ is the force exerted by the μ-th sphere in j direction [29]. The Eq. (7) includes the well-known Rotne–Prager tensor [32]. It describes that the flow velocity in i direction at point $\boldsymbol{x}$ is generated by the forces in all directions exerted on all spheres.

The Eq. (7) is used to iteratively calculate the flow field under no-slip boundary condition on sphere surface [9]. Remember this Rotne–Prager tensor is only valid for large values of r (*i.e.* $2a/r \ll 1$), otherwise we need to add more terms to the expansion. In fact, for widely separated spheres, the no-slip boundary condition is weakened in the iterative calculations. Only the centers of spheres, not all the surface elements of the colloidal spheres, are required to satisfy the no-slip boundary conditions in our calculations, and the results using this approximation show very good agreement with the theoretical formula in the following. The idea behind these iterative computational procedures is actually the reflection methods [33, 34, 35]. By iterations, a series of corrections are applied to the flow field due to the presence of suspended particles.

Once the necessary flow fields have been calculated, the total force exerted by the fluid on all the spheres can be summed as $F_i = -\sum_\mu F_{\mu i}$. In the following, a is the length unit, $6\pi\eta u_0 a$ is the force unit.

3. Hydrodynamic interactions between two identical spheres

Based on the above approximations, we consider two spheres with the same radius a in uniform creeping flow u_0 in Fig. 2. When the fluid flow along the x direction, Fig. 2 shows the lift force (F_y) perpendicular to the flow direction and the drag force (F_x) along the flow direction, respectively. Although only two spheres in fluid, there is force component perpendicular to the flow direction. The distance effect has different influences on the two kinds of forces. For the lift force, it decreases gradually with the increasing distance between them, and it is zero for sufficiently long distance. However, the drag force increases with the increment of the distance, naturally, it should be twice as much as the drag force, $6\pi\eta u_0 a$ [29], of a single sphere in the same uniform flow. Indeed, Fig. 2 (b) shows $F_x = 2 \times 6\pi\eta u_0 a$ for long enough distance, which indicates the very good matches between our iterative results and the theoretical force formula.

An important property of the hydrodynamic interactions is directional anisotropy [36]. In order to analyze the influences on the lift force and drag force of the different orientations of the connection lines between two spheres, we change positions of the two spheres along the dashed white line circle to keep the middle point of the line connecting centers of the two spheres at

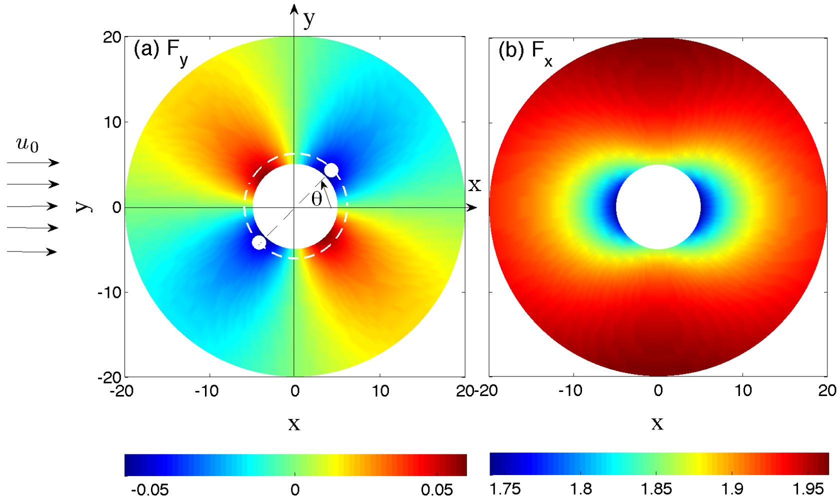

Fig. 2. The lift force F_y (a) and drag force F_x (b) on two spheres exerted by the uniform flow u_0 for different distances r and angles θ. r is the distance between two spheres' centers, and ranges from 10 to 40. θ is the angle between the flow direction and the connection line between two spheres. The flow is along the $+x$ direction and $u_0 = 1$. The two solid white circles denote two spheres with the same radius a. The dashed white line circle with a radius of 6 will be used to explore the relation of drag force and lift force to θ in Fig. 3.

the origin of the coordinate system in Fig. 2. The distance $r = 12$ (*i.e.*, the circle's radius is 6). The corresponding lift force and drag force profiles as functions of angle θ are plotted in Fig. 3. The lift force can be along with either $+y$ direction or $-y$ direction. Seen from Fig. 2 (a) and Fig. 3 (a), it gets the maximum value at $\theta = 45^{\circ}$ and 225° in the $-y$ direction, and the maximum value at $\theta = 135^{\circ}$ and 315° in the $+y$ direction. The drag force, as is well known, is always along the flow direction. Seen from Fig. 2 (b) and Fig. 3 (b), it has the maximum value at $\theta = 90^{\circ}$ and 270°, the minimum value at $\theta = 0^{\circ}$ and 180°.

The dependences of the lift force and drag force on distance r and angle θ can be fitted by the following formula

$$F_y(r, \theta) = -0.663 \frac{\sin 2\theta}{r}, \tag{8a}$$

$$F_x(r, \theta) = 2 - \frac{2.105}{r} - 0.663 \frac{\cos 2\theta}{r}. \tag{8b}$$

The dashed lines in Fig. 3 show the fitted results using the above formula at distance $r = 12$, which is corresponding to the dashed line circle in Fig. 2. It is shown that the fitted formula match well with the calculated results.

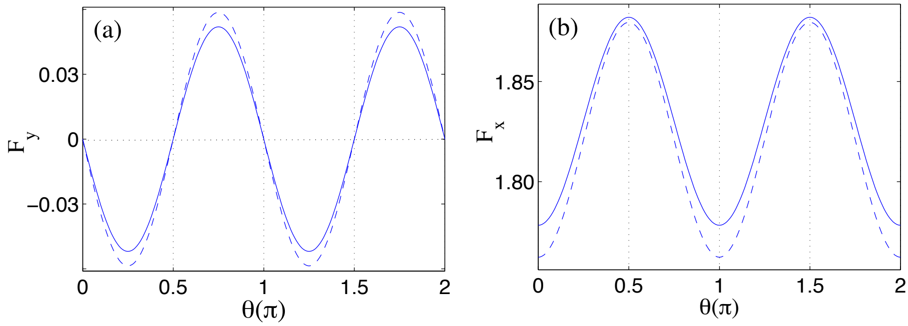

Fig. 3. The dependences of lift force F_y (a) and drag force F_x (b) on θ for the fixed distance $r = 12$, which corresponds to the dashed line circle in Fig. 2. The solid lines are calculated results and the dashed lines are fitted results using Eq. (8).

4. Conclusions

For low Reynolds number of flow, directly from the exact fluid velocity formula of uniform flow past a sphere, we have given a new, simpler and perhaps optimized derivation of the Rotne–Prager tensor to describe the hydrodynamic interactions between particles.

For the hydrodynamics of two identical spheres in uniform flow, we have given the more detailed results about the lift force and drag force profiles for different distances and direction angles of their connection lines, furthermore, given the fitted analytical force formula. The lift force can be along with either $+y$ direction or $-y$ direction depending on different angles θ. The results of lift force here provide the fundamental physical reasons to the chiral objects separation phenomenon in shear flow.

In the iterative computation procedures, we well simplify the no-slip boundary conditions on all surface elements of sphere by one point of sphere center. Our computational results show good agreement with theoretical formula. It should be kept in mind that this approximation works pretty well only for particle distances larger than $r \approx 3a$ [9]. Based on the current methods, it is naturally extended to formulate the real rigid chiral objects, which is currently underway.

The treatment of hydrodynamics under the framework of the Oseen or Rotne–Prager tensors is appropriate for dilute systems capturing only the far-field, pairwise hydrodynamic effects. However, in crowded biological systems and colloidal environments, the many-body hydrodynamic interactions [19] and lubrication forces may play a significant role in diffusion.

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