CLUSTERING OF CHIRAL PARTICLES IN FLOWS WITH BROKEN PARITY INVARIANCE

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Abstract The dynamics of small particles suspended in turbulent flows is an important problem in Nature and in Science. Previous work has mainly focused on the motion of spherical particles, while less is known about particles with asymmetric shapes. We study particles which break parity invariance (chiral particles). Particles of different chirality may respond differently to the structures of the flow. Helicoidal-like structures in the flow affect the particles differently depending on the parity of the helicoid as well as on the chirality of the particle. For flows where one of the two parities of the helicoidal-like structures is more common suspended chiral particles experience different levels on clustering depending on their chirality. Using analytical methods and direct numerical simulations we investigate the mechanisms of preferential sampling and clustering of chiral particles in flows with local or global breaking of parity invariance.

CHIRAL PARTICLES

One of the simplest examples of particles which break parity invariance are 'isotropic helicoids', first studied by Kelvin [6]. Just as spherical particles, isotropic helicoids have diagonal resistance -and moment of inertia tensors. But unlike spherical particles they have a coupling between the translational and rotational degrees of freedom. The motion of a small isotropic helicoid with velocity $\boldsymbol{v}$ and angular velocity $\boldsymbol{\omega}$ is governed by the force $\boldsymbol{F}$ and torque $\boldsymbol{\tau}$ [5]

$$\begin{aligned} \boldsymbol{F} &= m\dot{\boldsymbol{v}} = C^{\rm tt}(\boldsymbol{u}-\boldsymbol{v}) + C^{\rm tr}(\boldsymbol{\Omega}-\boldsymbol{\omega}) \\ \boldsymbol{\tau} &= I_0\dot{\boldsymbol{\omega}} = C^{\rm tr}(\boldsymbol{u}-\boldsymbol{v}) + C^{\rm rr}(\boldsymbol{\Omega}-\boldsymbol{\omega})\,. \end{aligned} \tag{1}$$

Here m and I_0 are the mass and moment of inertia of the particle, $\boldsymbol{u}$ is the flow velocity at the particle position and $\boldsymbol{\Omega} \equiv \boldsymbol{\nabla} \wedge \boldsymbol{u}/2$ is half the vorticity of the flow. The diagonal components of the resistance tensors, $C^{\rm tt}$ and $C^{\rm rr}$, and the parity-breaking coupling, $C^{\rm tr}$, are all scalar parameters. When $C^{\rm tr} = 0$, Eqs. (1) simplify to Stokes equations for a spherical particle. When $C^{\rm tr} \neq 0$, the equations are no longer invariant under parity transformations: if the spatial coordinates change sign, the terms proportional to $C^{\rm tr} \neq 0$ change sign relative to all other terms.
A second example of a parity-breaking particle is a rigid asymmetric particle consisting of four beads, as illustrated in Fig. 1**a** and **b**. The equations of motion for the four-bead particle can be obtained using the methods in Ref. [2]. Unlike spherical particles and isotropic helicoids, the center of mass of the asymmetric four-bead particle does not follow the streamlines of the flow in the limit of no particle inertia.
The local helicity $H(\boldsymbol{r})$ of a fluid flow can be expressed in terms of the alignment between the fluid velocity, $\boldsymbol{u}$, and the vorticity of the flow, $2\boldsymbol{\Omega}$, i.e. $H \equiv 2\boldsymbol{u}\cdot\boldsymbol{\Omega}$. It is expected that particles of different chiralities (different sign of $C^{\rm tr}$ in Eq. (1), or the mirror images in Fig. 1**a** and **b**) behave differently depending on the sign and magnitude of H. To illustrate the asymmetry between the particles in Fig. 1**a** and **b**, their trajectories are plotted in Fig. 1**c** for a helicoidal flow, $\boldsymbol{u} = (-5y, 5x, 1)$ and $\boldsymbol{\Omega} = (0, 0, 5)$. If the helicoidal flow in Fig. 1**c** is mirrored in the origin, the role of the red and green particles is interchanged.

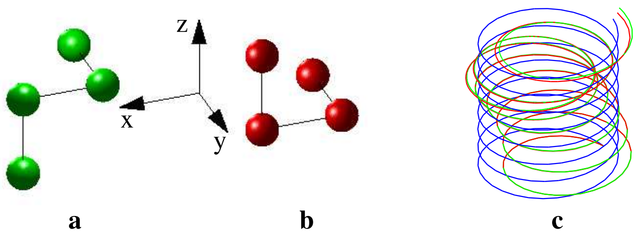

Figure 1. a, **b**: Asymmetric particles consisting of four well-separated beads with two different chiralities. The relative positions and orientations of the beads are kept fixed by infinitesimally thin rods. **c**: Inertialess motion of the particles in a simple helicoid, $\boldsymbol{u} = (-5y, 5x, 1)$. One streamline of the flow $\boldsymbol{u}$ is shown as a blue line. Even though the particles lack inertia, their center of mass can not follow the streamlines. The particle trajectories are shown as green for particle **a** and red for particle **b**.

FLOWS WITH LOCAL OR GLOBAL BREAKING OF PARITY INVARIANCE

Particles of different chirality move differently through the flow, allowing them to sample different flow regions. If the flow is reflection invariant, it is as likely to find a specific helical structure as it is to find its mirror image. This implies that there is no major difference between trajectories of particles with different chiralities: the only difference is a reflection of the flow. Homogeneous isotropic turbulence is reflection invariant, and the magnitude of clustering and preferential sampling is thus, on average, independent of the particle chirality. Due to boundary conditions, or due to the nature of the forcing of the turbulence, reflection invariance is often broken in systems encountered in nature and in applications. In flows with broken parity invariance helical structures with one sign of the local helicity H is more common than the other sign. As a net effect, particles may show different statistical properties depending on their chiralities.

We study the motion of chiral particles in DNS of turbulent flows, as well as in model flows in which one sign of the helicity is more likely. One example of such flow is the Arnold-Beltrami-Childress (ABC) flow [1]

$$\boldsymbol{u} = (C\cos y + A\sin z, A\cos z + B\sin x, B\cos x + C\sin y)\,. \tag{2}$$

This flow has $\boldsymbol{\Omega} = \boldsymbol{u}/2$ which implies a positive helicity $H = |\boldsymbol{u}|^2$. A second method to construct a reflection-breaking model flow is to project out and remove the modes of a flow which contributes to the undesired sign of H [7].

We address the questions on which regions of the flow are preferentially sampled by chiral particles and how the chiral particles cluster. We discuss the similarities and differences between isotropic helicoids (1) and the four-bead model (Fig. 1) for both reflection invariant flows and the reflection-breaking flows mentioned above. We compare our results to previous results on clustering of spherical particles in reflection-invariant flows, see for instance Ref. [4], and in rotating flows [3].

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