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Clustering of chiral particles in flows with broken parity invariance

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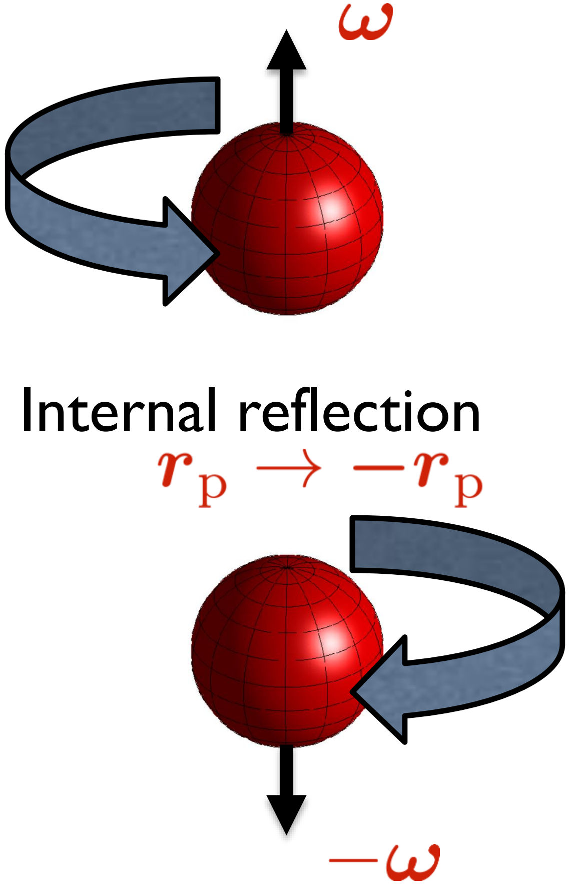
Spherical particle

Equations for velocity $\boldsymbol{v}$ and angular velocity $\boldsymbol{\omega}$ for small spherical particle at position $\boldsymbol{r}$: Happel & Brenner, Low Reynolds number hydrodynamics (1963)

$$\dot{\boldsymbol{v}} = \frac{1}{\tau_{\rm p}}\left[\boldsymbol{u}(\boldsymbol{r},t) - \boldsymbol{v}\right]$$

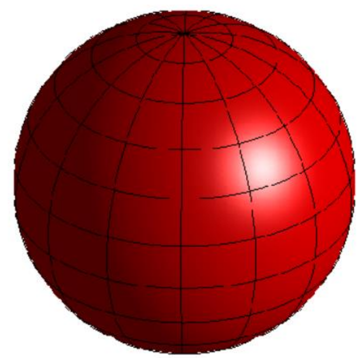
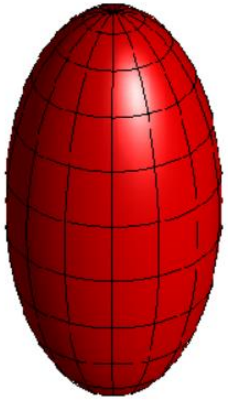
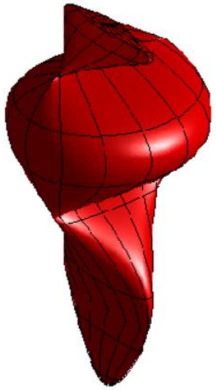
$$\dot{\boldsymbol{\omega}} = \frac{1}{\tau_{\rm p}}\left[\frac{10}{3}(\boldsymbol{\Omega}(\boldsymbol{r},t) - \boldsymbol{\omega})\right]$$



- $\boldsymbol{u}$ Fluid velocity
- $\boldsymbol{\Omega}$ Half fluid vorticity
- $\tau_{\rm p}$ Particle relaxation time

Dynamics statistically invariant under rotations and reflections if $\boldsymbol{u}$ statistically invariant under rotations and reflections

Particle symmetries

Rotation invariance / Reflection invariance	✓	✗
✓		
✗	**'Isotropic helicoid'** (this talk)	

Example of an isotropic helicoid

Recipe from Lord Kelvin:

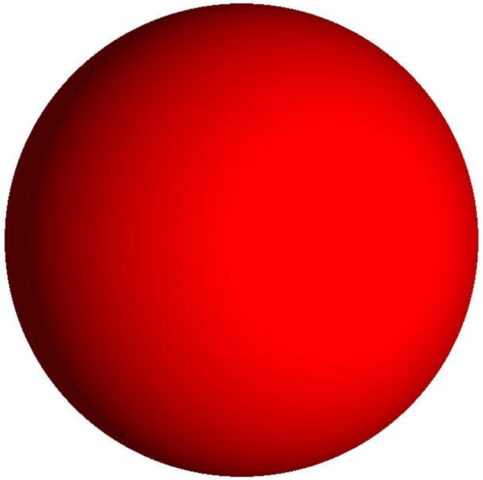
"An isotropic helicoid can be made by attaching projecting vanes to the surface of a globe in proper positions; for instance cutting at 45º each, at the middles of the twelve quadrants of any three great circles dividing the globe into eight quadrantal triangles."

Kelvin, Phil. Mag. **42** (1871)

Example of an isotropic helicoid

Recipe from Lord Kelvin (1884)

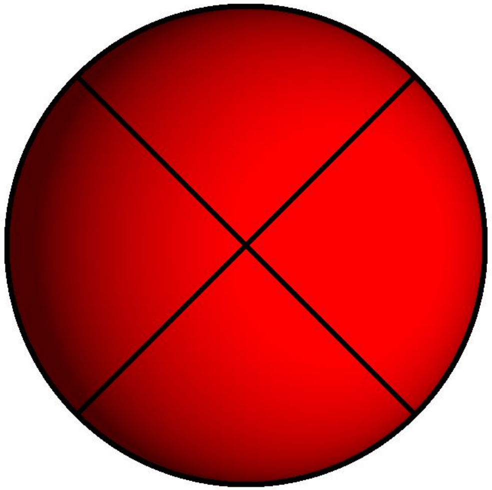
Start with a sphere



Example of an isotropic helicoid

Recipe from Lord Kelvin (1884)

✓ Start with a sphere
Draw 3 great circles

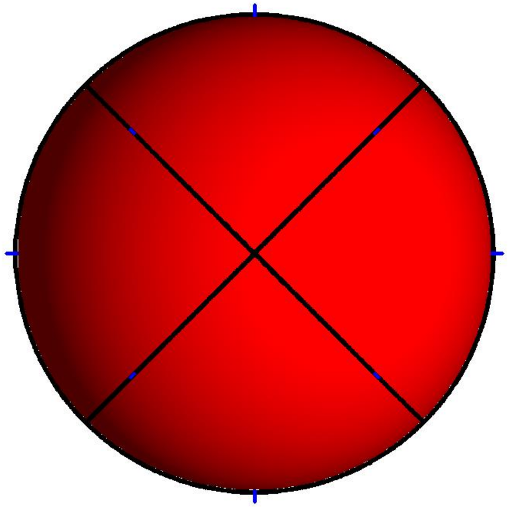


Example of an isotropic helicoid

Recipe from Lord Kelvin (1884)

- ✓ Start with a sphere
- ✓ Draw 3 great circles

Identify 12 vane positions at midpoints of quarter-arcs

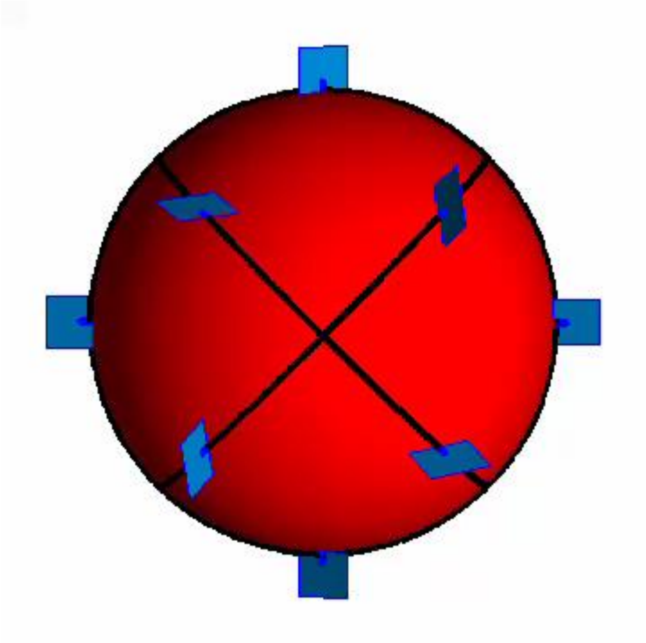


Example of an isotropic helicoid

Recipe from Lord Kelvin (1884)

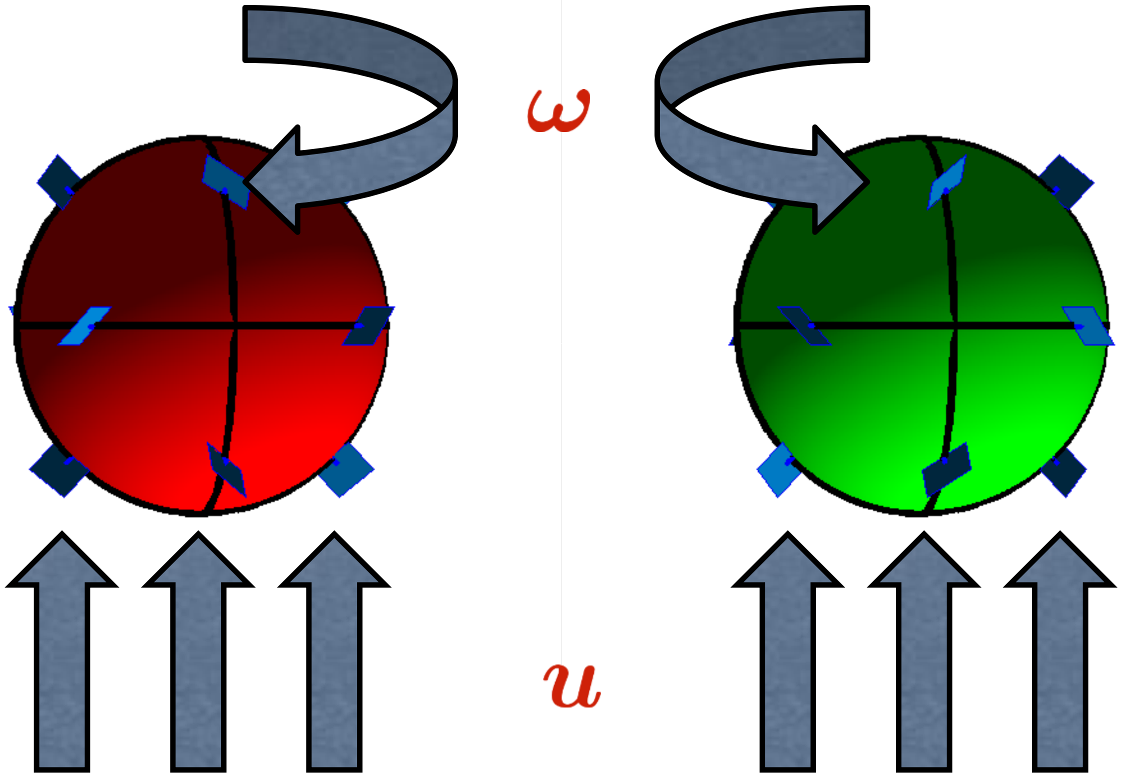
- ✓ Start with a sphere
- ✓ Draw 3 great circles
- ✓ Identify 12 vane positions at midpoints of quarter-arcs

Put a vane on each vane position (45° to arc line)



Chirality

In a constant flow $\boldsymbol{u}$, the isotropic helicoid starts spinning around the flow direction with angular velocity $\boldsymbol{\omega}$.
The spinning direction depends on the chirality of the vanes.



Left handed $C_0 < 0$ *Right handed* $C_0 > 0$

Motion of an 'isotropic helicoid'

Equations for velocity $\boldsymbol{v}$ and angular velocity $\boldsymbol{\omega}$ for small isotropic helicoid:

Happel & Brenner, Low Reynolds number hydrodynamics (1963)

$$\dot{\boldsymbol{v}} = \frac{1}{\tau_{\mathrm{p}}}\left[\boldsymbol{u}(\boldsymbol{r},t) - \boldsymbol{v} + \frac{2a}{9}C_0(\boldsymbol{\Omega}(\boldsymbol{r},t) - \boldsymbol{\omega})\right]$$

$$\dot{\boldsymbol{\omega}} = \frac{1}{\tau_{\mathrm{p}}}\left[\frac{10}{3}(\boldsymbol{\Omega}(\boldsymbol{r},t) - \boldsymbol{\omega}) + \frac{5}{9a}C_0(\boldsymbol{u}(\boldsymbol{r},t) - \boldsymbol{v})\right]$$

Stokes' law   translation – rotation coupling (scalar)

$a = \sqrt{5I_0/(2m)}$ Particle 'size' (defined by mass m and moment of inertia I_0)

C_0 Helicoidality

Ratio of rotational and translational inertia fixed to that of sphere

Equations break spatial reflection symmetry ($\boldsymbol{\omega}$ pseudovector)

Dimensionless parameters

Stokes number $\mathrm{St} \equiv \frac{\tau_\mathrm{p}}{\tau_\eta}$ Size $\overline{a} \equiv \frac{a}{\eta}$ Helicoidality C_0

with τ_η and η smallest time- and length scales of flow.

Dynamics may grow indefinitely unless $-\sqrt{27} < C_0 < \sqrt{27}$.

St and $\overline{a}$ constrained by particle density higher than that of the fluid and geometrical size must be smaller than η .

Simulations and theory is done using a random single-scale flow characterised by the Kubo number

$$\mathrm{Ku} \equiv \frac{u_0 \tau_\eta}{\eta}$$

with u_0 typical speed of flow.

Clustering at small St

Expand compressibility of particle-velocity field $\boldsymbol{\nabla}\cdot\boldsymbol{v}$ in small $\mathrm{St}\sim\tau_\mathrm{p}$

$$\boldsymbol{\nabla}\cdot\boldsymbol{v} = -\frac{27}{27-C_0^2}\tau_\mathrm{p}\left[\mathrm{Tr}\left(\boldsymbol{\nabla}\boldsymbol{u}^\mathrm{T}\boldsymbol{\nabla}\boldsymbol{u}^\mathrm{T}\right) - \frac{1}{15}\mathrm{aC_0}\mathrm{Tr}\left(\boldsymbol{\nabla}\boldsymbol{u}^\mathrm{T}\boldsymbol{\nabla}\boldsymbol{\Omega}^\mathrm{T}\right)\right]$$

Centrifuge effect with modified amplitude
Maxey, J. Fluid Mech. **174** (1987)

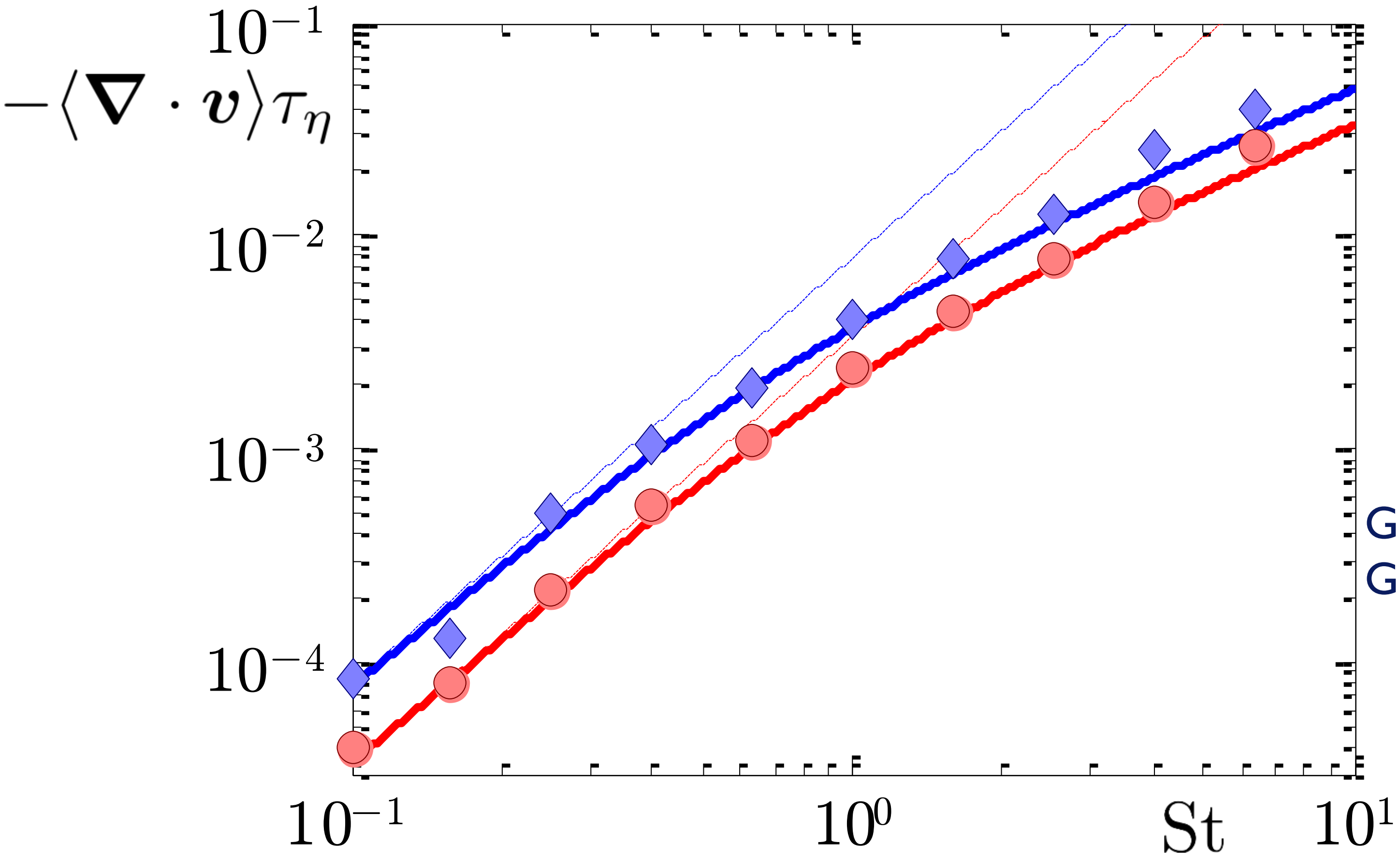
Term due to parity breaking of system

Reflection-invariant systems have $\langle\mathrm{Tr}\left(\boldsymbol{\nabla}\boldsymbol{u}^\mathrm{T}\boldsymbol{\nabla}\boldsymbol{\Omega}^\mathrm{T}\right)\rangle = 0$

Isotropic helicoids violate that relation $\langle\mathrm{Tr}\left(\boldsymbol{\nabla}\boldsymbol{u}^\mathrm{T}\boldsymbol{\nabla}\boldsymbol{\Omega}^\mathrm{T}\right)\rangle \propto \tau_\mathrm{p}\mathrm{C_0}$

$\Rightarrow$ In a parity-invariant isotropic flow clustering does not depend on sign of C_0

Clustering at small St in random flow



$$\mathrm{Ku} \equiv \frac{u_0 \tau_\eta}{\eta} = 0.1$$

$$\overline{a} = 1$$

Small-Ku theory
Gustavsson & Mehlig EPL **96** (2011)
Gustavsson & Mehlig arXiv:1412.4374 (2014)

Small-St limit

$$\langle \nabla \cdot v \rangle \tau_\eta \sim -\frac{27\,\mathrm{Ku}^4\,\mathrm{St}^2(1800 + 7\,\overline{a}^2 C_0^2)}{20(27 - C_0^2)^2}$$

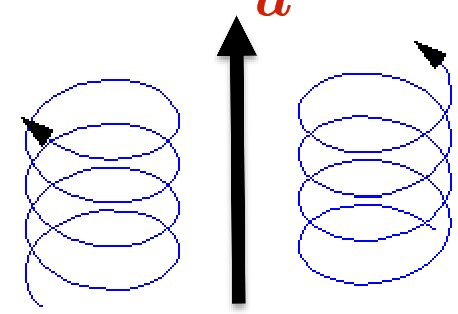
Spherical particle ($C_0 = 0$)

Isotropic helicoid ($C_0 = 3$ or $C_0 = -3$)

Where do particles go?

Inertial particles sample the flow preferentially (e.g. spiral out if vortices)

Local helicity $H \equiv 2\boldsymbol{u} \cdot \boldsymbol{\Omega}$



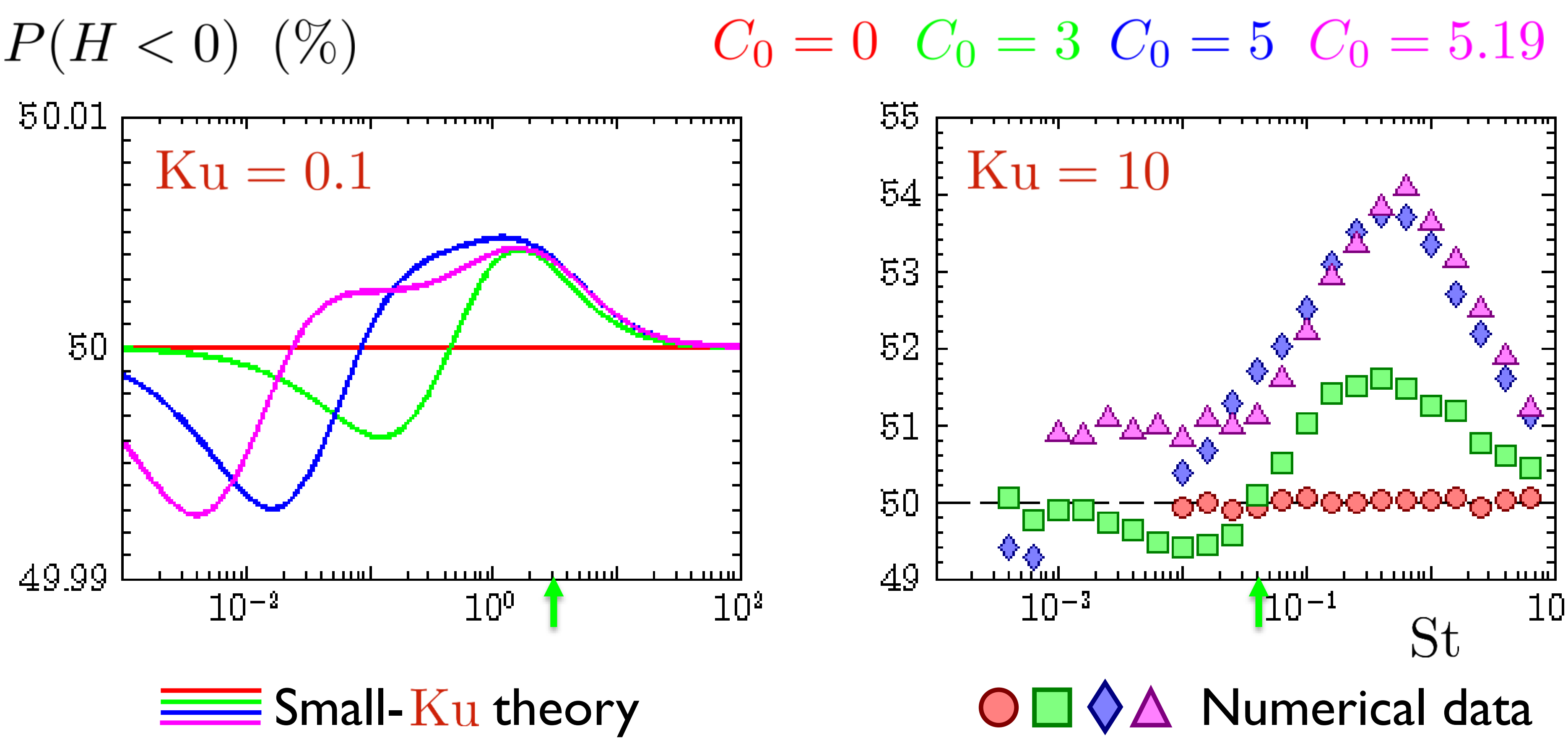
Moments $\langle H^n \rangle$

Distribution $P(H)$

Probability to be in region with negative helicity

$$P(H<0) = 0.5 + \overline{a}\, C_0\, \mathrm{Ku}^2\, \mathrm{St} \times \frac{15\sqrt{5}(50C_0^4 - 729(10+3\,\mathrm{St})(-5+\mathrm{St}(5+6\,\mathrm{St})) + 135C_0^2(-20+\mathrm{St}(7+15\,\mathrm{St})))}{2\pi(5C_0^2 - 27(1+2\,\mathrm{St})(5+3\,\mathrm{St}))(10C_0^2 - 27(1+\mathrm{St})(10+3\,\mathrm{St}))^2}$$

Probability of negative helicity



$$P(H < 0) = 0.5 + \overline{a}\, C_0\, \mathrm{Ku}^2\, \mathrm{St}$$

$$\times \frac{15\sqrt{5}(50C_0^4 - 729(10 + 3\,\mathrm{St})(-5 + \mathrm{St}(5 + 6\,\mathrm{St})) + 135C_0^2(-20 + \mathrm{St}(7 + 15\,\mathrm{St})))}{2\pi(5C_0^2 - 27(1 + 2\,\mathrm{St})(5 + 3\,\mathrm{St}))(10C_0^2 - 27(1 + \mathrm{St})(10 + 3\,\mathrm{St}))^2}$$

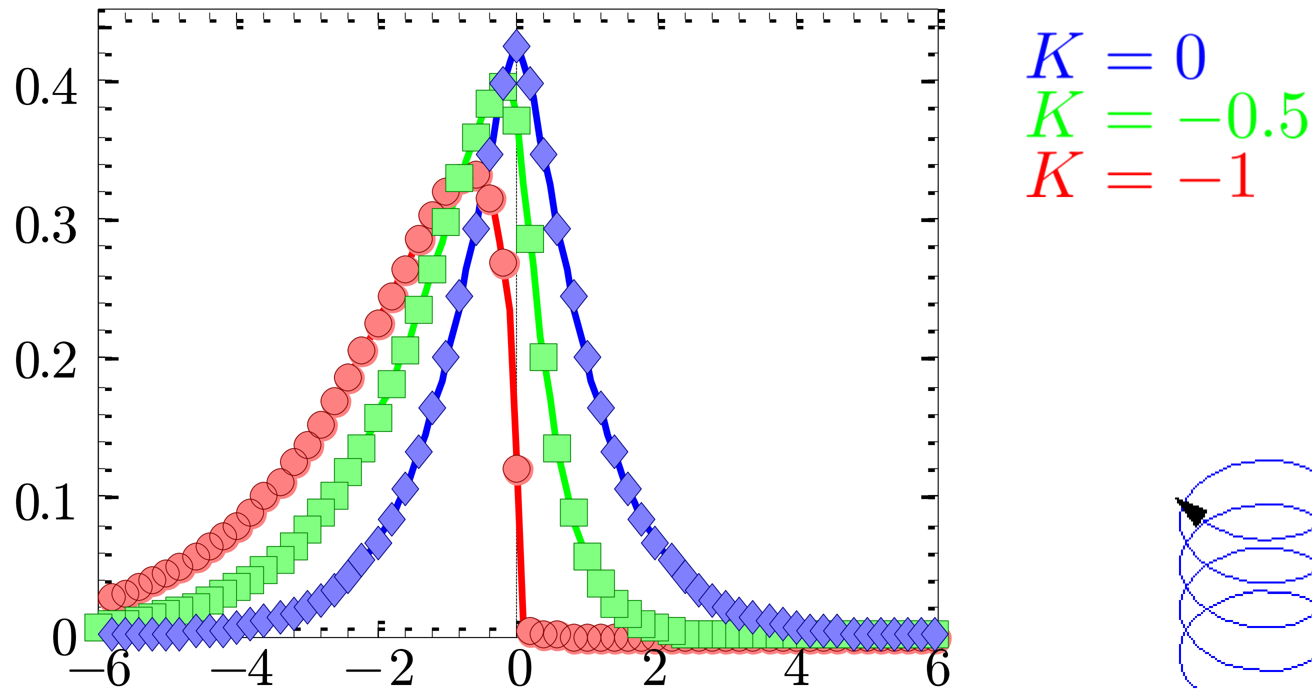
Flow with helical asymmetry

Break parity invariance of flow by removing selected Fourier modes

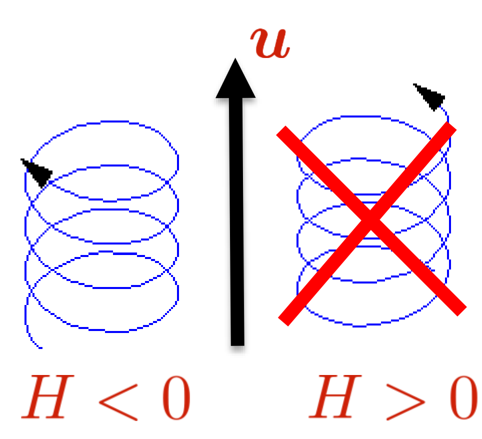
Mussacchio, Biferale & Toschi, J. Fluid Mech. **730** (2013)

Helicity parameter K

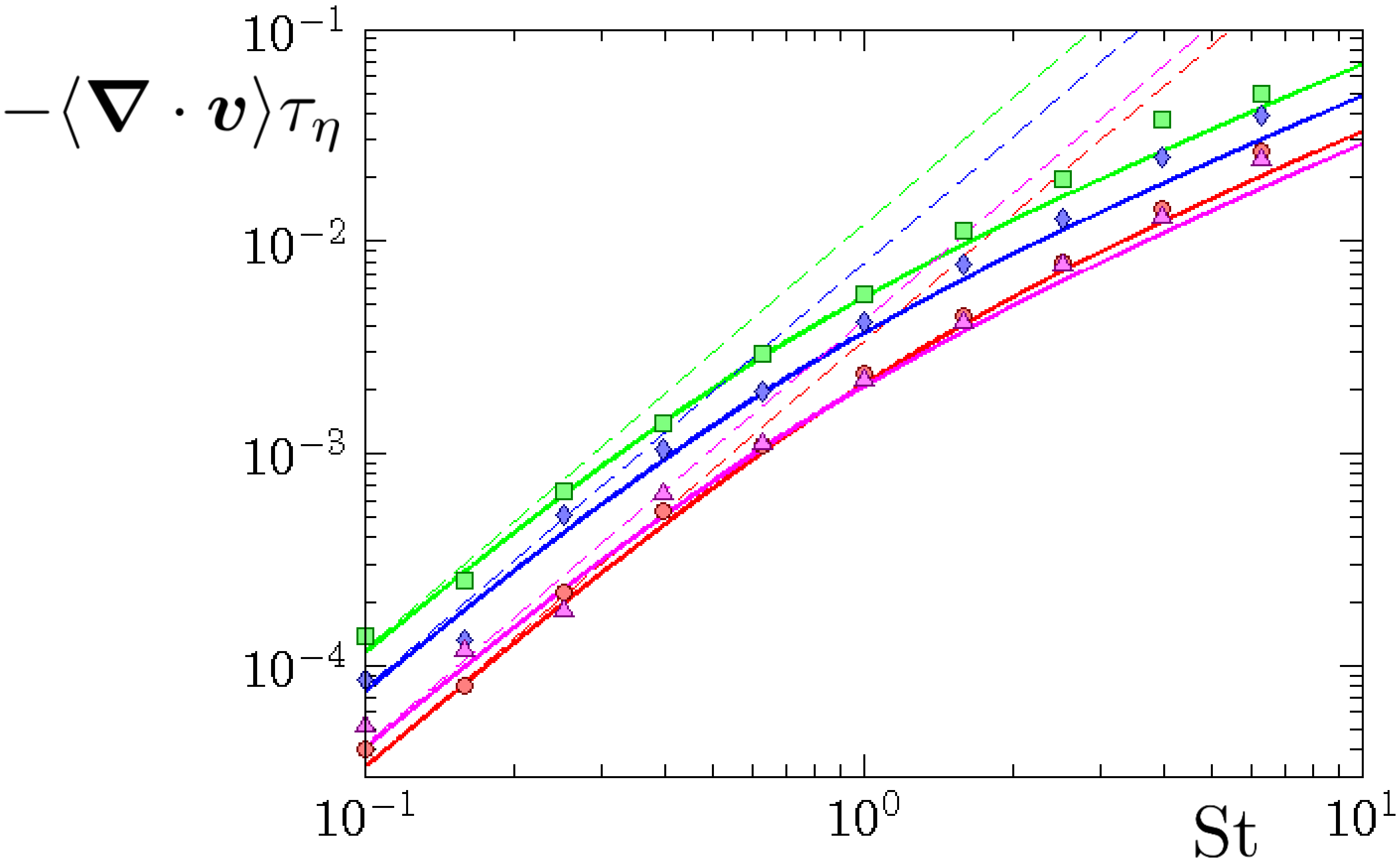
- $K > 0$ Right-handed structures ($H = 2\boldsymbol{u} \cdot \boldsymbol{\Omega} > 0$) more common
- $K < 0$ Left-handed structures ($H = 2\boldsymbol{u} \cdot \boldsymbol{\Omega} < 0$) more common



Probability density of flow helicity H



Clustering at small St in random flow



$$\mathrm{Ku} \equiv \frac{u_0 \tau_\eta}{\eta} = 0.1$$

$$\overline{a} = 1$$

Small-Ku theory

Gustavsson & Mehlig EPL **96** (2011)

Small-St limit

- ○ Spherical particle ($C_0 = 0$) in neutral flow ($K = 0$)
- □ Right-handed particle ($C_0 = 3$) in left-handed flow ($K = -1$)
- ◇ Right-handed particle ($C_0 = 3$) in neutral flow ($K = 0$)
- △ Right-handed particle ($C_0 = 3$) in right-handed flow ($K = 1$)

Conclusions

Isotropic helicoids are rotation invariant particles which break reflection invariance (two chiralities)

Coupling between translational and rotational degrees of freedom changes dynamics compared to spherical particles (modified clustering, preferential sampling etc.)

The two chiralities may show different dynamics if the particle size is not too small and flow is persistent

Flows with broken parity invariance increase the differences in the dynamics of the two particles