Max Planck Institute for the Physics of Complex Systems

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Modelling fluctuations in granular materials: dense suspensions

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Key Points

Granular materials are characterized by a non-affine motion and often by anisotropy

Can we determine particles non-affine motion by employing equilibrium?

Can we predict anisotropy by employing equilibrium?

Dense Suspensions

Particles (hard spheres) in a Newtonian fluid

Neutrally buoyant suspensions
(the densities of the spheres and suspending fluid are equal)

Reynolds number based on particle size

$$Re_p = \frac{\rho \dot{\gamma} a^2}{\mu} \doteq 0$$

Viscous Forces dominate over the Inertial Forces

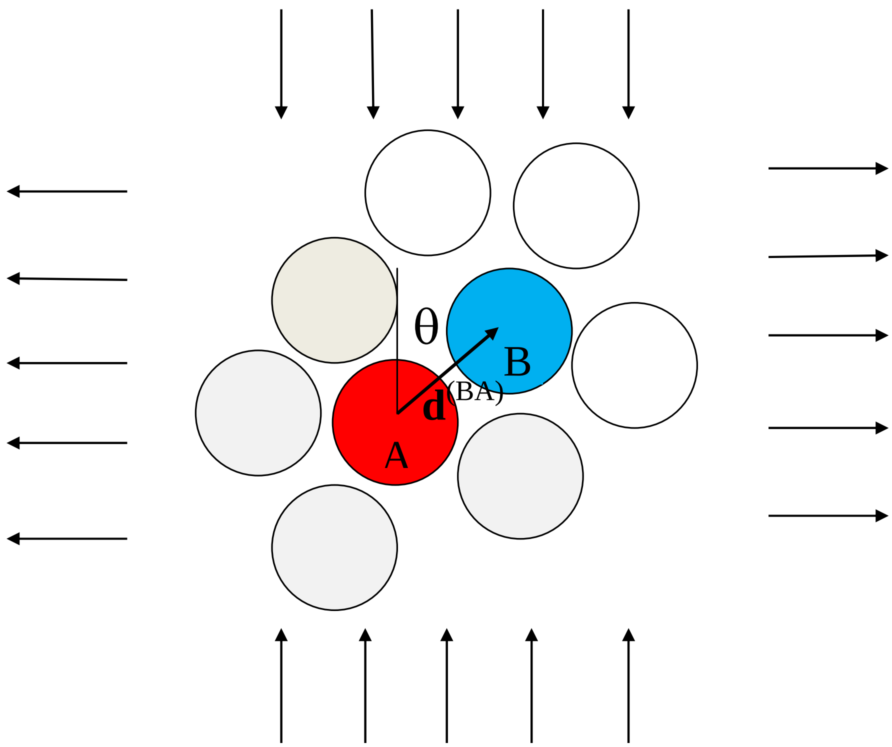
Goal

Employ equilibrium for a typical pair

Prediction of particle trajectories

Prediction of microstructure: particle distribution

Pure Shearing



Theoretical Model

1. Kinematics

2. Force

3. Equilibrium

4 Statistics

5. Stress

Kinematics A-B

Relative velocity of centers

$$v_\alpha^{(BA)} = \dot{s}^{(BA)}\hat{d}_\alpha^{(BA)} + 2a\dot{\theta}^{(BA)}\hat{t}_\alpha^{(BA)}$$

$$d_\alpha = (2a + s)\hat{d}_\alpha$$

a is the particle radius

s is the smallest separation between particles edges

Kinematics A-n

The relative velocity spheres A and n follows the affine motion

$$(2a + s)\, D_{\beta\gamma}\hat{d}_\gamma^{(nA)}$$

Force

Viscous Force + Repulsive Force
(Jeffrey and Onishi, 1983, JFM)

Interaction B-A

$$F_\alpha^{(BA)} = 6\pi\mu a K_{\alpha\beta}^{(BA)} v_\beta^{(BA)} - \frac{F_0}{s^{(BA)}} \hat{d}_\alpha^{(BA)}$$

$$-9.54\pi\mu a^2 \left(\hat{t}_\beta D_{\beta\xi} \hat{d}_\xi\right) \hat{t}_\alpha^{(BA)}$$

where

$$K_{\alpha\beta}^{(BA)} = \frac{1}{4}\frac{a}{s^{(BA)}} \hat{d}_\alpha^{(BA)} \hat{d}_\beta^{(BA)} + \left[\frac{1}{6}\ln\left(\frac{a}{s^{(BA)}}\right) + 0.64\right] \hat{t}_a^{(BA)} \hat{t}_\beta^{(BA)}$$

Essential Ingredients

$$F_\alpha^{(BA)} = F_N^{(BA)} \hat{d}_\alpha^{(BA)} + F_T^{(BA)} \hat{t}_\alpha^{(BA)} - \frac{F_0}{s^{(BA)}} \hat{d}_\alpha^{(BA)}$$

$$F_N^{(BA)} \propto \frac{\dot{s}^{(BA)}}{s^{(BA)}}$$

$$F_T^{(BA)} \propto \log\left(\frac{a}{s^{(BA)}}\right) \dot{\theta}^{(BA)}$$

Interaction n-A

$$F_{\alpha}^{(nA)} = \frac{3}{\bar{s}} a^2 \pi \mu \left(D_{\beta\xi} \hat{d}_{\xi}^{(nA)} \hat{d}_{\beta}^{(nA)} \right) \hat{d}_{\alpha}^{(nA)} - \frac{F_0}{\bar{s}} \hat{d}_{\alpha}^{(nA)}$$

$$+ a^2 \pi \mu \left[2 \ln \left(\frac{a}{\bar{s}} \right) - 1.92 \right] \left(D_{\beta\xi} \hat{t}_{\xi}^{(nA)} \hat{d}_{\beta}^{(nA)} \right) \hat{t}_{\alpha}^{(nA)}$$

Equilibrium

Equilibrium particle A

$$F_\alpha^{(BA)} + \sum_{n \neq B}^{N^{(A)}} F_\alpha^{(nA)} = 0$$

$$\sum_{n \neq B}^{N^{(A)}} F_\alpha^{(nA)} = \frac{3}{\bar{s}} a^2 \pi \mu D_{\beta\xi} \sum_{n \neq B}^{N^{(A)}} \hat{d}_\xi^{(nA)} \hat{d}_\beta^{(nA)} \hat{d}_\alpha^{(nA)}$$

$$+ a^2 \pi \mu \left[2 \ln \left(\frac{a}{\bar{s}} \right) - 1.92 \right] D_{\beta\xi} \sum_{n \neq B}^{N^{(A)}} \hat{t}_\xi^{(nA} \hat{d}_\beta^{(nA)} \hat{t}_\alpha^{(nA)}$$

$$- \frac{F_0}{\bar{s}} \sum_{n \neq B}^{N^{(A)}} \hat{d}_\alpha^{(nA)}$$

Equilibrium particle B

Interchanging A with B

$$\mathbf{d}^{(AB)} = -\mathbf{d}^{(BA)}$$

Structural Sums

From local tensors...

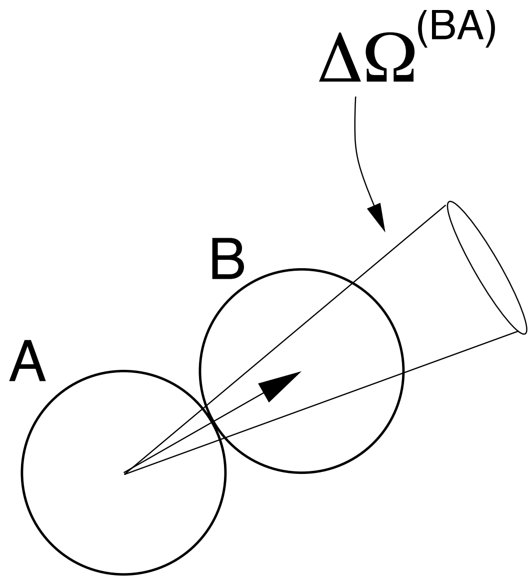
$$\sum_{n \neq B}^{N^{(A)}} \hat{d}_{\alpha}^{(nA)} \hat{d}_{\beta}^{(nA)} \hat{d}_{\xi}^{(nA)}$$

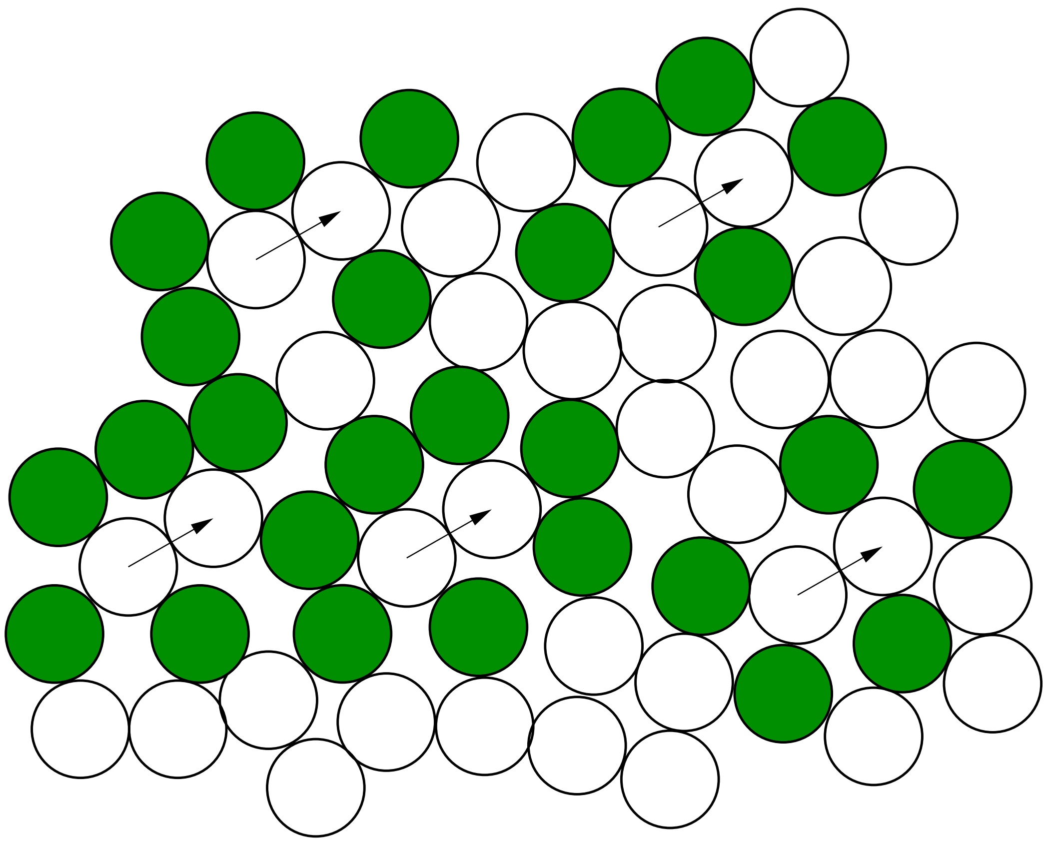
$$\sum_{n \neq B}^{N^{(A)}} \hat{d}_{\alpha}^{(nA)}$$

...to global (average) tensors

Conditional Average

All pairs B-A with orientation near $\hat{d}^{(BA)}$


ΔΩ(BA)
B
A



Assume the neighbors are uniformily distributed about the pair A-B

$$J_{\xi\alpha\beta}^{(BA)} = \overline{\sum_{n\neq B}^{N^{(A)}} \hat{d}_{\xi}^{(nA)} \hat{d}_{\alpha}^{(nA)} \hat{d}_{\beta}^{(nA)}}$$

$$= \eta_1 \hat{d}_i^{(BA)} \hat{d}_j^{(BA)} \hat{d}_k^{(BA)} + \eta_2 (\delta_{ij} \hat{d}_k^{(BA)} + \delta_{ik} \hat{d}_j^{(BA)} + \delta_{kj} \hat{d}_i^{(BA)})$$

$$Y_{\alpha}^{(BA)} = \overline{\sum_{n\neq B}^{N^{(A)}} \hat{d}_i^{(nA)}} = \zeta \hat{d}_{\alpha}^{(BA)}$$

$$\eta_1 = 0$$

$$\eta_2 = -3\sqrt{3}(k-1)/(16\pi)$$

$$\zeta = -3\sqrt{3}(k-1)/(4\pi)$$

k is average number of near contacts per particle

Sum up

For every pair A-B

Equilibrium Equations

$$0 = 6\pi\mu a K^{(BA)}_{\alpha\beta} v^{(BA)}_{\beta} + \ldots + \frac{3}{\bar{s}} a^2 \pi\mu J_{\xi\beta\alpha} D_{\beta\alpha} - \frac{F_0}{\bar{s}} Y_{\alpha} + \ldots$$

$$J_{\xi\beta\alpha} D_{\beta\alpha} = \eta_1 \hat{d}^{(BA)}_{\alpha} \hat{d}^{(BA)}_{\beta} \hat{d}^{(BA)}_{\xi} D_{\beta\alpha}$$

$$+\eta_2 (\delta_{\alpha\beta} \hat{d}^{(BA)}_{\xi} + \delta_{\xi\alpha} \hat{d}^{(BA)}_{\beta} + \delta_{\xi\beta} \hat{d}^{(BA)}_{\alpha}) D_{\beta\alpha}$$

Solution depends on the orientation of the pair $\hat{\mathbf{d}}^{(\mathbf{BA})}$ with respect to $\mathbf{D}$

Next Step

Take the components of the force balance parallel and perpendicular to the line of centeres $A - B$

Two Unknowns:

1) $\dot{s}^{(BA)}$

2) $\dot{\theta}^{(BA)}$

Two Equilibrium Equations

Relative Motion in Pure Shear

Make s dimensionless with a and F_0 with $a^3\mu\dot{\gamma}$

Force balance along **d**

$$\dot{s} = \frac{ds}{d\gamma}$$

$$\frac{1}{s}\frac{ds}{d\gamma} = \frac{2}{3}F\left(\frac{1}{s} + \frac{\zeta}{\bar{s}}\right) + \frac{2\eta_2}{\bar{s}}\cos 2\theta$$

Force balance perpendicular to **d**

$$\dot{\theta} = \frac{d\theta}{d\gamma}$$

$$\frac{d\theta}{d\gamma} = -\frac{1}{2}\frac{[3\eta_2/\bar{s} - 4.77 + \zeta\ln(1/\bar{s}) - 0.96\zeta]}{\ln(1/s) + 3.81}\sin 2\theta$$

Circumferential Distribution $\mathscr{A}$

Steady State

Constant flux of the distribution along the trajectory

$$\frac{d}{d\sigma}(\dot{\sigma}\mathscr{A}) = 0$$

$\mathscr{A}(\sigma)d\sigma$ is the average number of particles in $d\sigma$

$$\dot{\sigma} = \left[\dot{s}^2 + (2+s)^2\dot{\theta}^2\right]^{1/2}$$

$$\frac{d\mathscr{A}}{d\gamma} = -\mathscr{A}\frac{d\dot{\sigma}}{d\gamma}\frac{1}{\dot{\sigma}}$$

Governing Equations

$$\frac{ds}{d\gamma} = \frac{2}{3}F\left(1 + \frac{s\zeta}{\bar{s}}\right) + \frac{2s\eta_2}{\bar{s}}\cos 2\theta$$

$$\frac{d\theta}{d\gamma} = -\frac{1}{2}\frac{[3\eta_2/\bar{s} - 4.77 + \zeta \ln(1/\bar{s}) - 0.96\zeta]}{\ln(1/s) + 3.81}\sin 2\theta$$

$$\frac{d\mathscr{A}}{d\gamma} = -\mathscr{A}\frac{d\dot{\boldsymbol{\sigma}}}{d\gamma}\frac{1}{\dot{\boldsymbol{\sigma}}}$$

recall

$$\dot{\sigma} = \left[\dot{s}^2 + (2+s)^2\dot{\theta}^2\right]^{1/2}$$

Numerical Predictions

Torquato (e.g. PRE, 1995)

$$\bar{s} = \frac{\sqrt{\pi}}{8G}$$

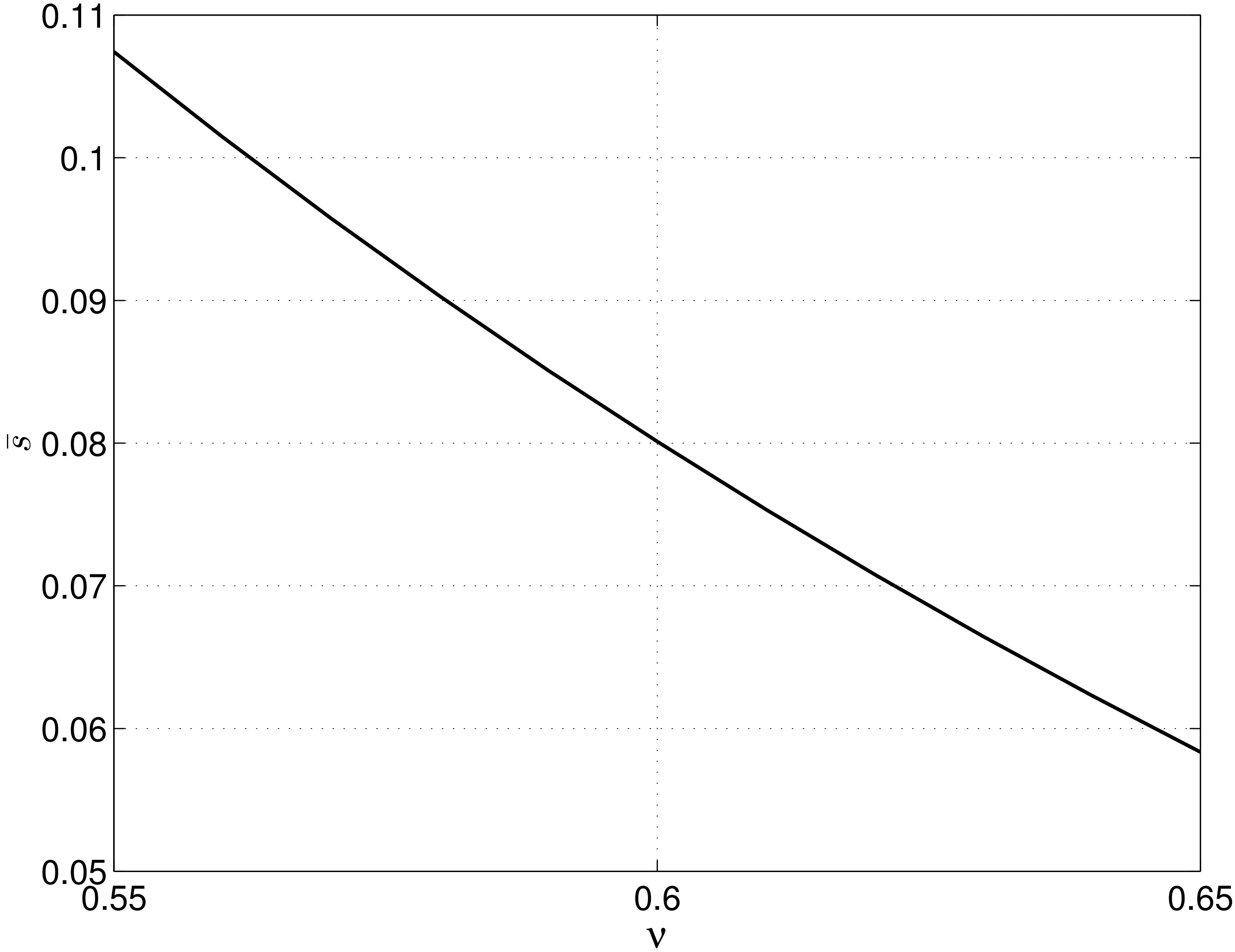
if $\nu < 0.69$

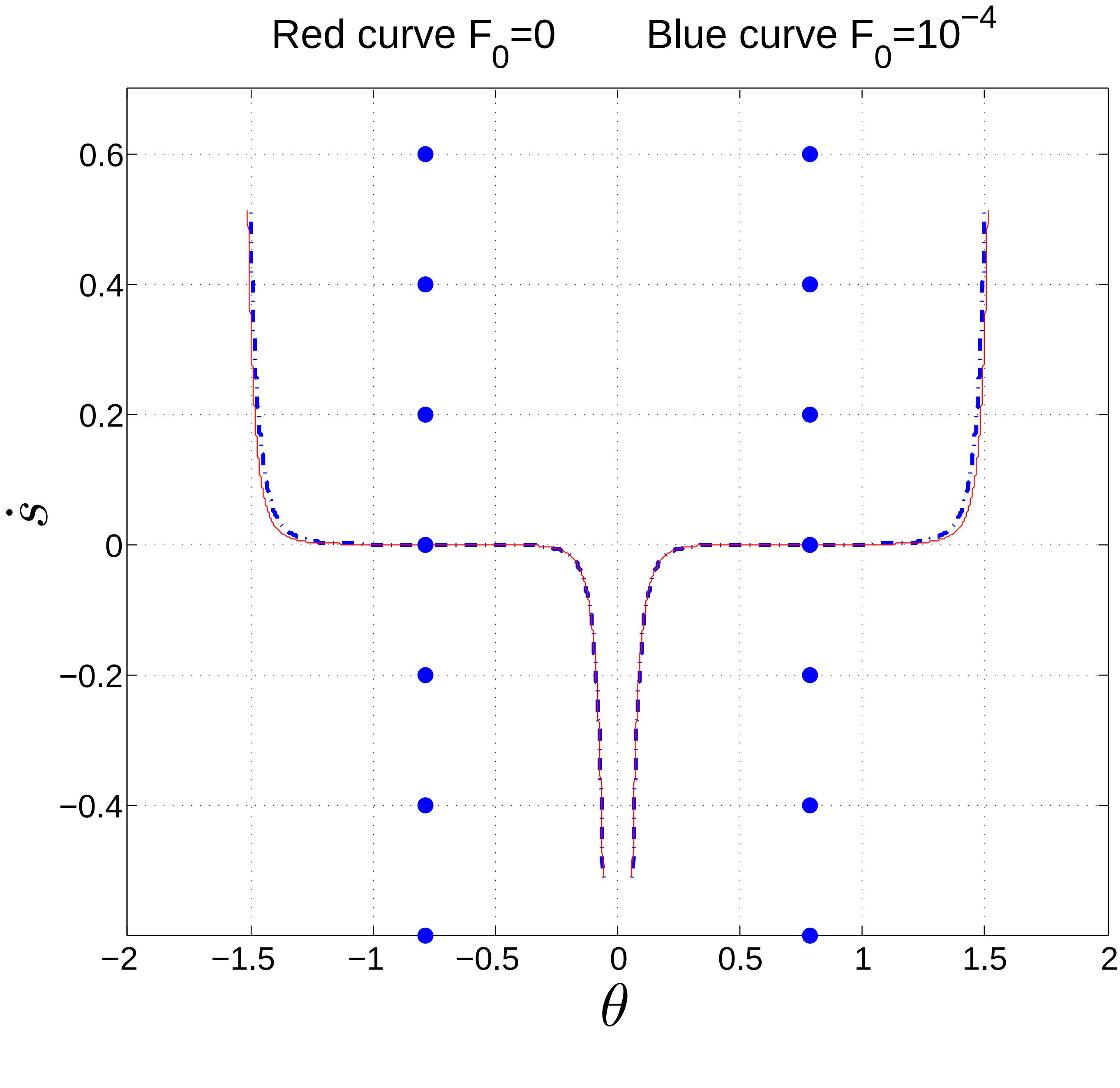
$$G = \frac{\nu \times (16 - 7\nu)}{16(1-\nu)^2}$$

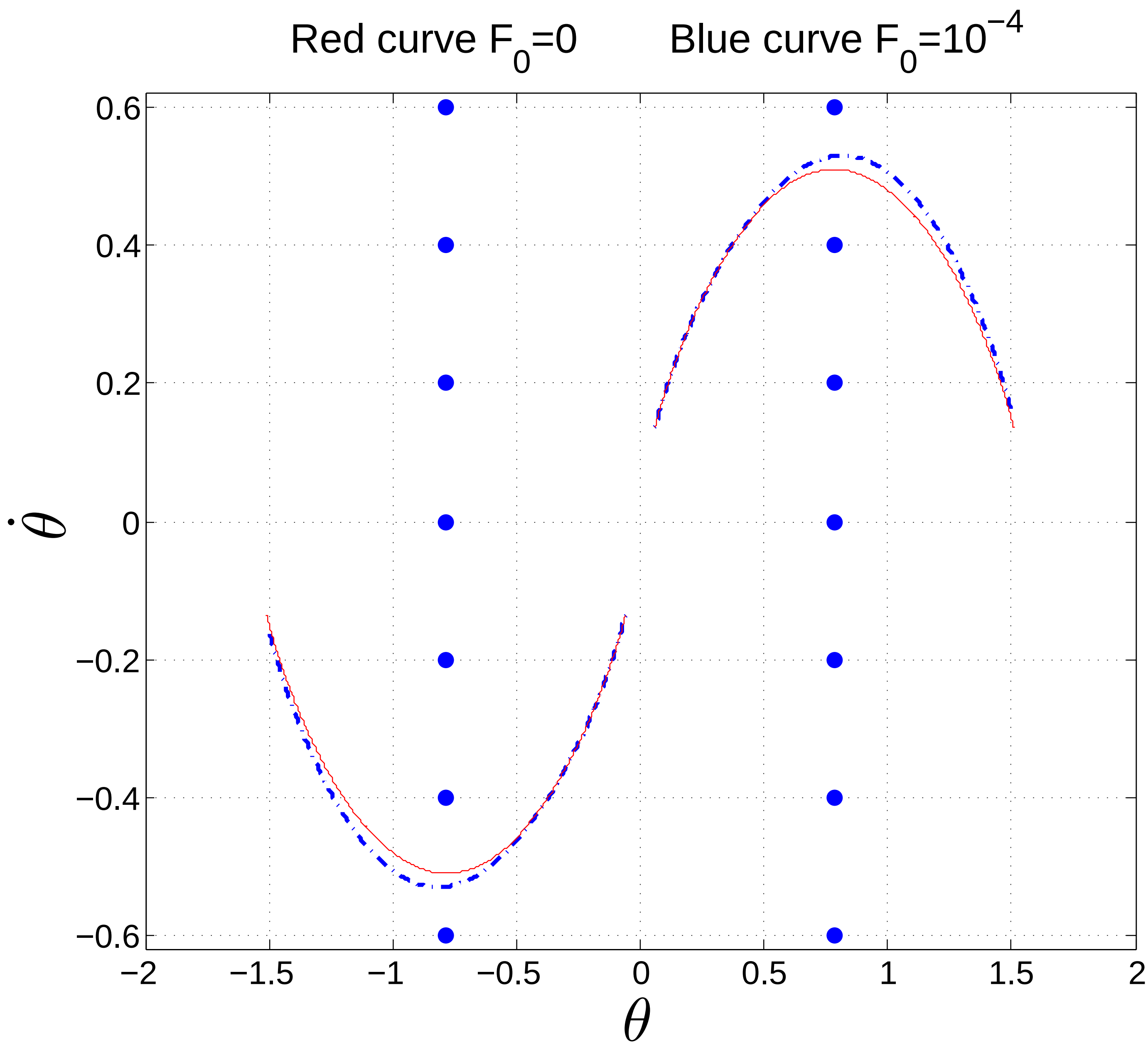
otherwise

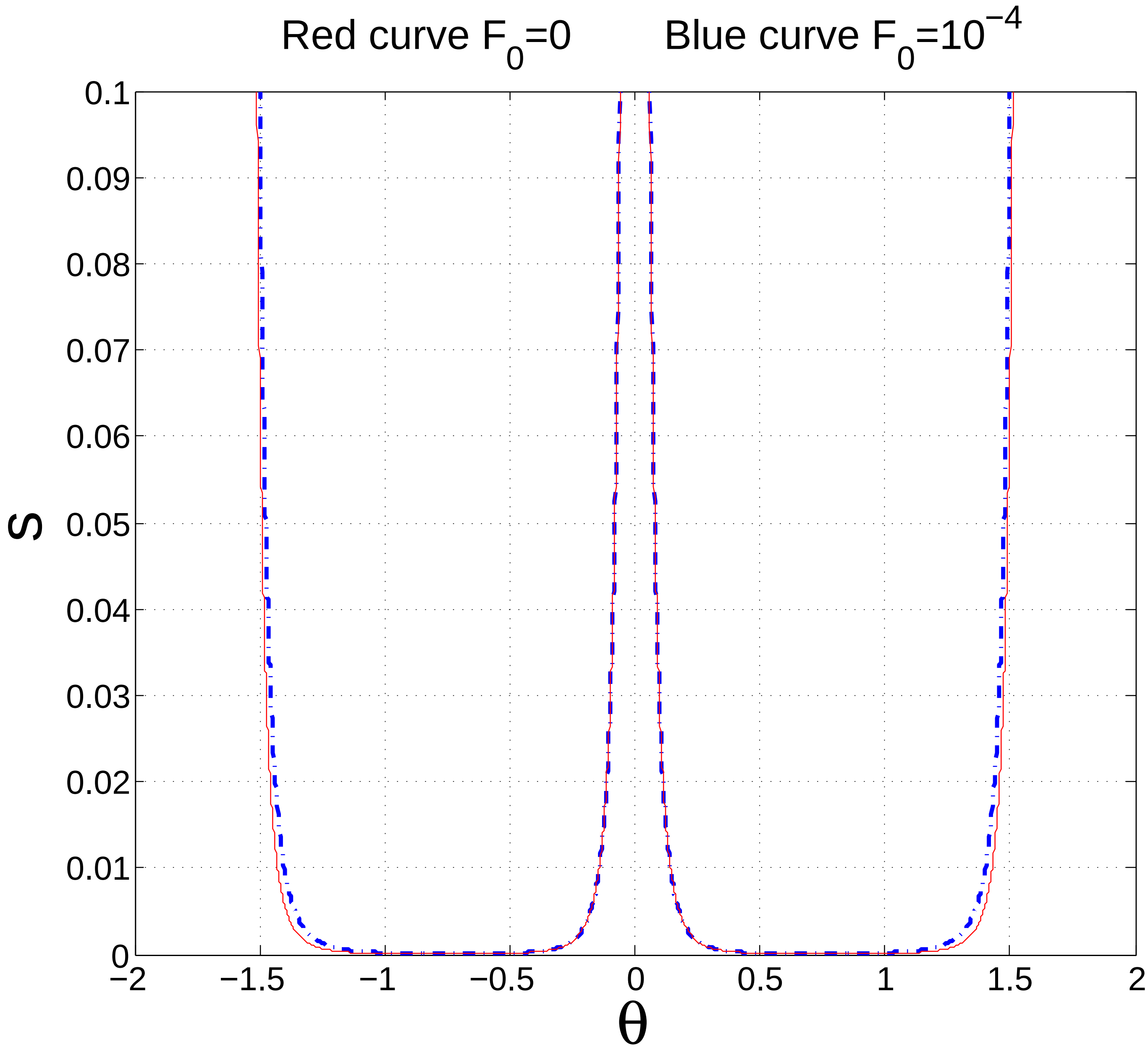
$$G = \nu \times 7.2646^{\frac{0.82-0.69}{0.82-\nu}}$$

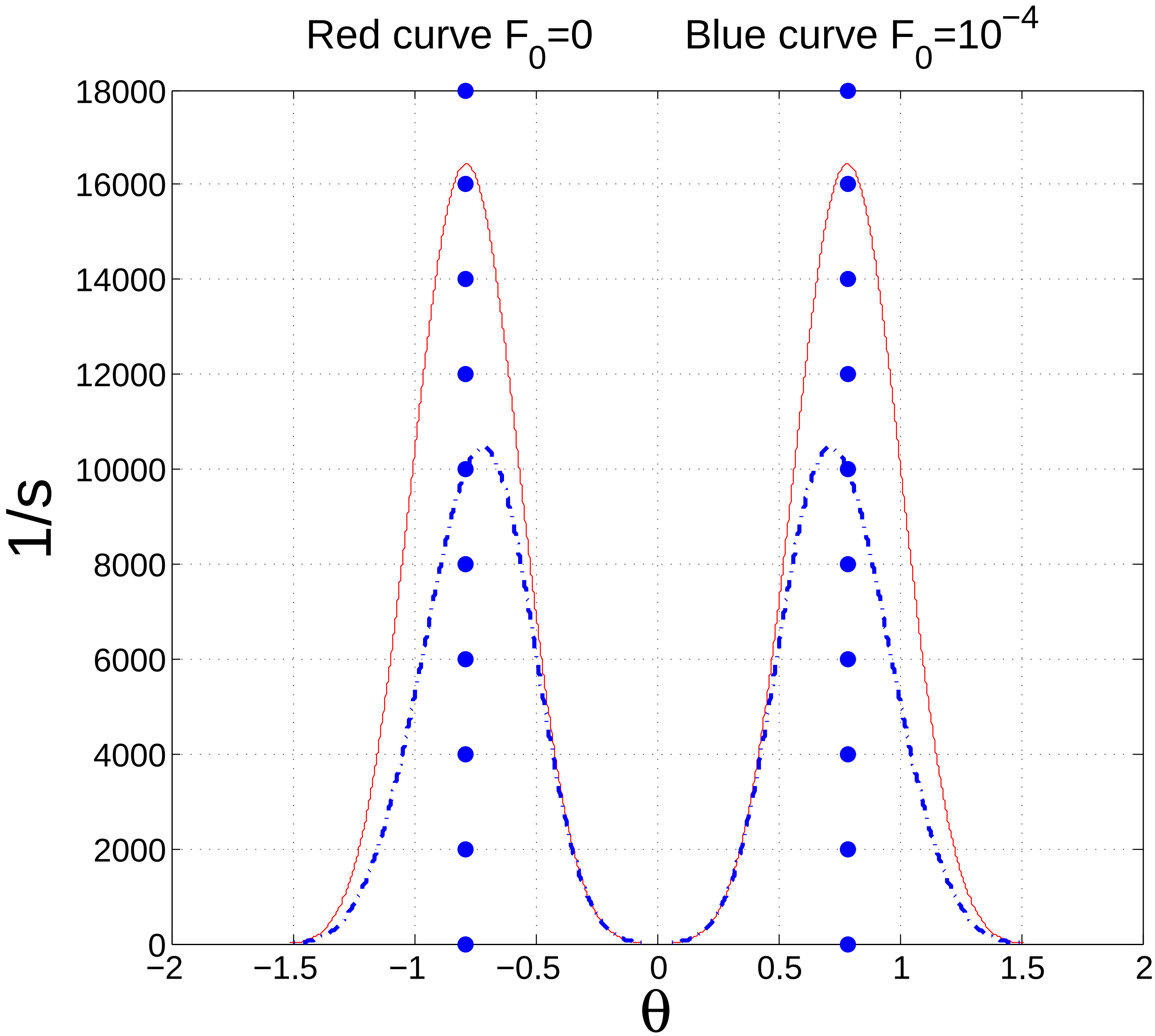
Average separation

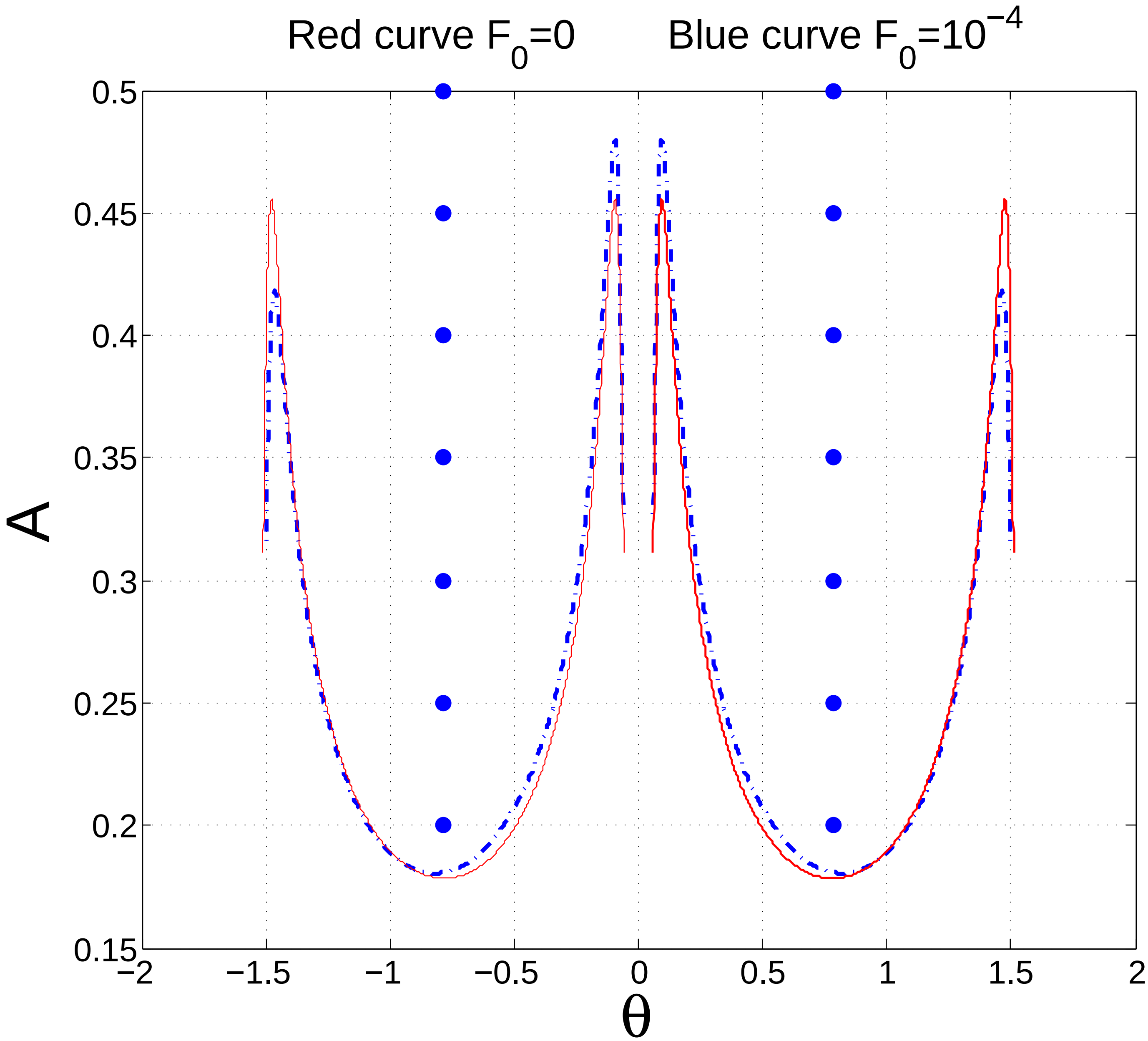



Red curve F_0=0 Blue curve F_0=10^{-4}
0.6
0.4
0.2
0
−0.2
−0.4
−2
−1.5
−1
−0.5
0
0.5
1
1.5
2
$\dot{s}$
θ


Red curve F_0=0   Blue curve F_0=10^{-4}
0.6
0.4
0.2
0
−0.2
−0.4
−0.6
$\dot{\theta}$
−2
−1.5
−1
−0.5
0
0.5
1
1.5
2
θ


Red curve F_0=0 Blue curve F_0=10^{-4}
S
θ
0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
−2
−1.5
−1
−0.5
0
0.5
1
1.5
2

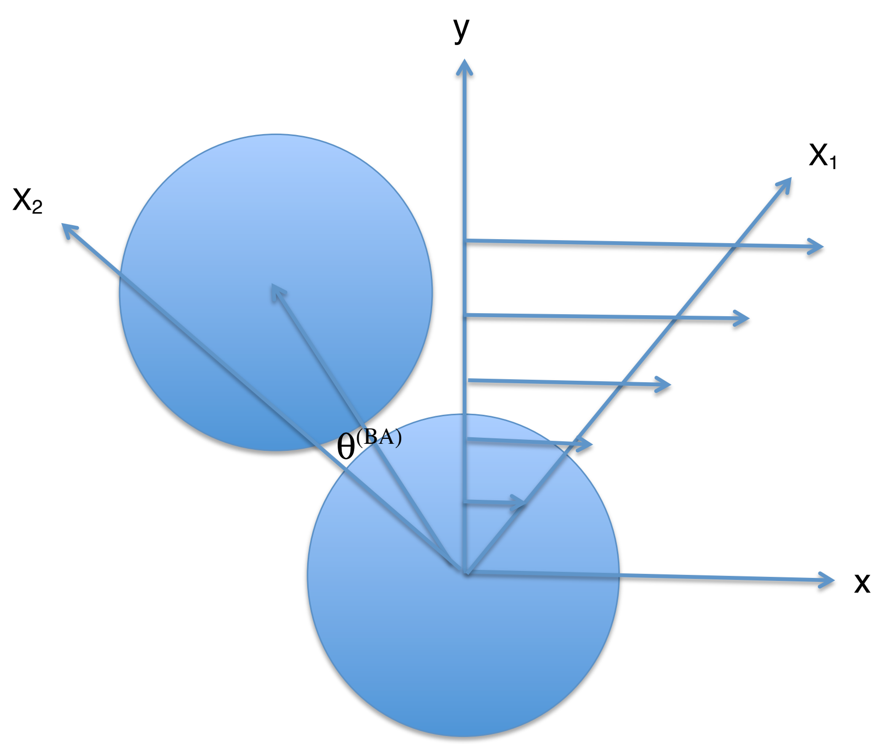

Red curve F0=0
Blue curve F0=10−4
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
1/s
−2
−1.5
−1
−0.5
0
0.5
1
1.5
2
θ



Red curve F_0=0
Blue curve $F_0=10^{-4}$
A
θ
0.5
0.45
0.4
0.35
0.3
0.25
0.2
0.15
−2
−1.5
−1
−0.5
0
0.5
1
1.5
2

Simple Shear

J.T. Jenkins and L. La Ragione, JFM, **763**, 2015



Kinematics A-B

Relative velocity of “contact points”

$$v_{\alpha}^{(BA)} + 2a\Omega^{\times}\hat{t}_{a}^{(BA)}$$

Relative velocity of centers

$$v_{\alpha}^{(BA)} = \dot{s}^{(BA)}\hat{d}_{\alpha}^{(BA)} + 2a\dot{\theta}^{(BA)}\hat{t}_{\alpha}^{(BA)}$$

Kinematics A-n

The velocity of the “contact points” of spheres *A* and *n* moving with the average translation and rotation

$$2a\left(D_{\beta\gamma} + W_{\beta\gamma}\right)\hat{d}_{\gamma}^{(nA)} + 2a\Omega^{\times}\hat{t}_{\beta}^{(nA)}$$

Equilibrium

Equilibrium particle A

$$F_{\alpha}^{(BA)} + \sum_{n \neq B}^{N^{(A)}} F_{\alpha}^{(nA)} = 0$$

$$\sum_{n \neq B}^{N^{(A)}} F_{\alpha}^{(nA)} = \frac{3}{\bar{s}} a^2 \pi \mu D_{\beta\xi} \sum_{n \neq B}^{N^{(A)}} \hat{d}_{\xi}^{(nA)} \hat{d}_{\beta}^{(nA)} \hat{d}_{\alpha}^{(nA)}$$

$$+ a^2 \pi \mu \left[2 \ln \left(\frac{1}{\bar{s}} \right) - 0.96 \right] \left(\Omega^{\times} - W^{\times} \right) \sum_{n \neq B}^{N^{(A)}} \hat{t}_{\alpha}^{(nA)}$$

$$+ a^2 \pi \mu \left[2 \ln \left(\frac{1}{\bar{s}} \right) - 1.92 \right] D_{\beta\xi} \sum_{n \neq B}^{N^{(A)}} \hat{t}_{\xi}^{(nA} \hat{d}_{\beta}^{(nA)} \hat{t}_{\alpha}^{(nA)}$$

$$- \frac{F_0}{\bar{s}} \sum_{n \neq B}^{N^{(A)}} \hat{d}_{\alpha}^{(nA)}$$

Equilibrium particle B
Interchanging A with B

$$\mathbf{d}^{(AB)} = -\mathbf{d}^{(BA)}$$

Next Step

Take the components of the force balance parallel and perpendicular to the line of centeres $A-B$

Three Unknowns:

1) $\dot{s}^{(BA)}$

2) $\dot{\theta}^{(BA)}$

3) $\Omega^{\times}$

Two Local Equilibrium Equations
and
One Global Equilibrium (Symmetry of the Stress)

Input k, $\bar{s}$ and $\mathbf{D}$, $\mathbf{W}^{\times}$

Relative Motion in Simple Shearing

Force balance along **d**

$$\dot{s} = \frac{ds}{d\gamma}$$

$$\frac{1}{s}\frac{ds}{d\gamma} = \frac{2}{3}F\left(\frac{1}{s} + \frac{\zeta}{\bar{s}}\right) + \frac{2\eta_2}{\bar{s}}\cos 2\theta$$

Force balance perpendicular to **d**

$$\dot{\theta} = \frac{d\theta}{d\gamma}$$

$$\frac{d\theta}{d\gamma} = -\frac{W^{\times}}{\dot{\gamma}} - \left[\frac{\ln(1/s) - 0.48}{\ln(1/s) + 3.81}\right]\frac{(\Omega^{\times} - W^{\times})}{\dot{\gamma}}$$

$$-\frac{[\zeta\ln(1/\bar{s}) - 0.48\zeta]}{\ln(1/s) + 3.81}\frac{(\Omega^{\times} - W^{\times})}{\dot{\gamma}}$$

$$-\frac{1}{2}\frac{[3\eta_2/\bar{s} - 4.77 + \zeta\ln(1/\bar{s}) - 0.96\zeta]}{\ln(1/s) + 3.81}\sin 2\theta$$

Dimensionless Equilibriated Force

$$\frac{F_{\alpha}^{(BA)}}{\pi a^2 \mu \dot{\gamma}} \propto \left[\frac{\dot{s}}{s};\;\; \log\left(\frac{1}{s}\right)\dot{\theta};\;\; \frac{F}{\bar{s}} \right]$$

Dimensionless Stress Tensor

$$t_{\alpha_\beta} = \frac{T_{\alpha\beta}}{a\mu\dot{\gamma}}$$

with

$$T_{\alpha_\beta} = 2na\int_{\sigma} \mathscr{A}\left(\boldsymbol{\sigma}\right) F_{\alpha}^{(BA)} \hat{d}_{\beta}^{(BA)} d\boldsymbol{\sigma}$$

Symmetry of the Stress

$$\varepsilon_{\alpha\beta} t_{\alpha\beta} = 0$$

$$\frac{\Omega^{\times} - W^{\times}}{\dot{\gamma}} = -\frac{\left[3\eta_2/\bar{s} + \xi \ln\left(1/\bar{s}\right) - 0.96\xi\right]}{k\xi\left[\ln\left(1/\bar{s}\right) - 0.48\right]} \int_{\hat{\gamma}} A\left(\boldsymbol{\sigma}\right) \sin 2\theta \frac{d\boldsymbol{\sigma}}{d\gamma} d\gamma$$

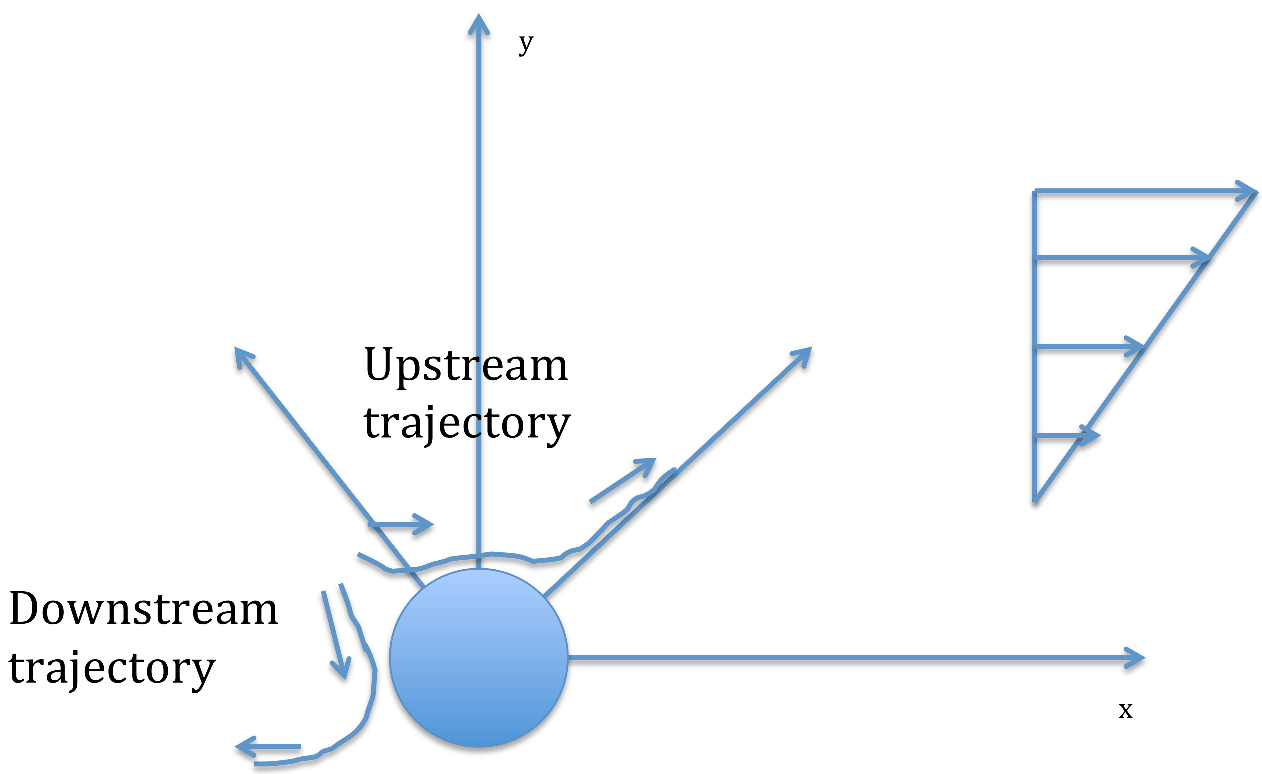
Circumferential Distribution $\mathscr{A}$

Constant Flux

$$\frac{d}{d\sigma}(\dot{\sigma}\mathscr{A}) = 0$$

$$\frac{d\mathscr{A}}{d\gamma} = -\mathscr{A}\frac{d\dot{\sigma}}{d\gamma}\frac{1}{\dot{\sigma}}$$

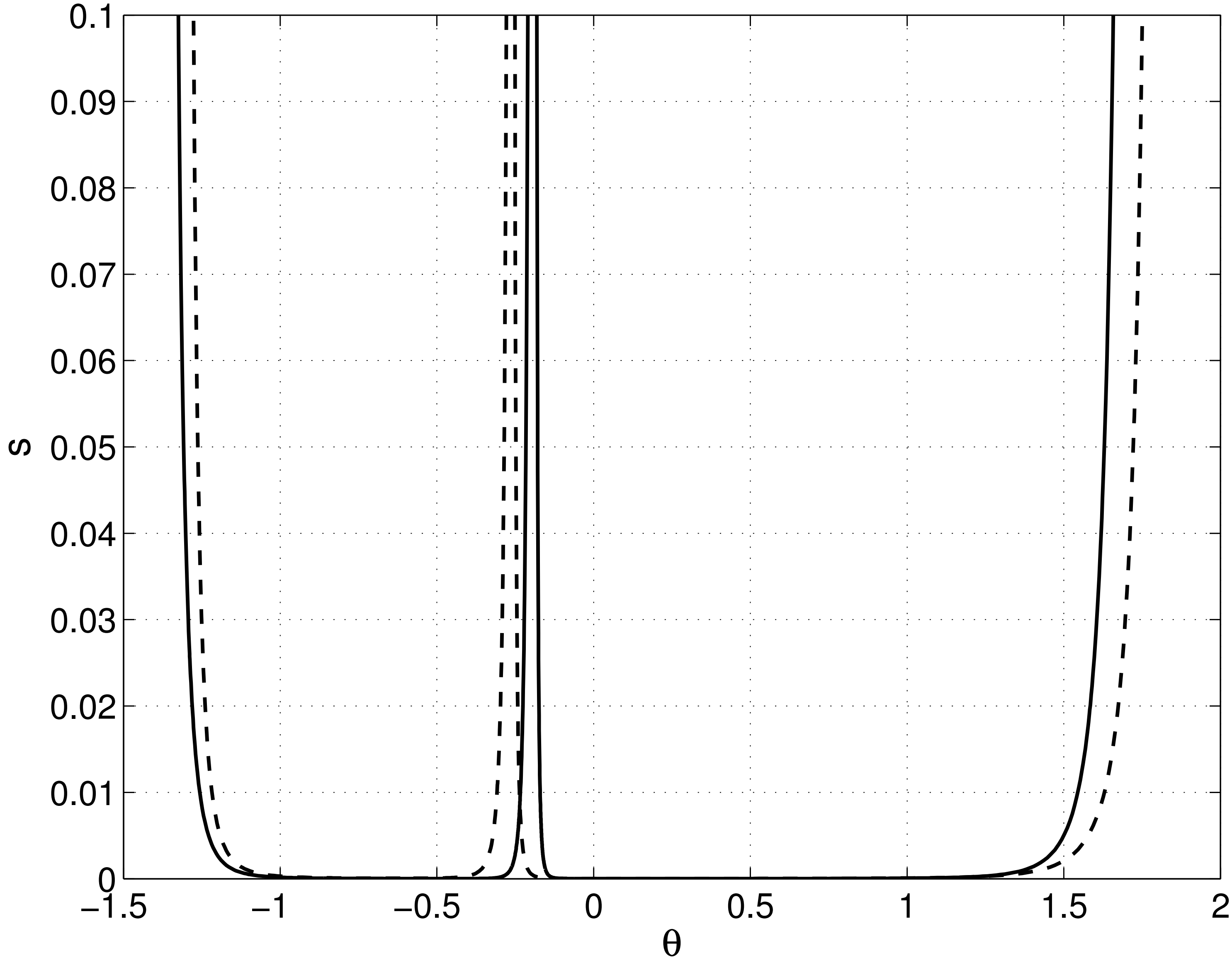
Representative trajectories s=s(θ)



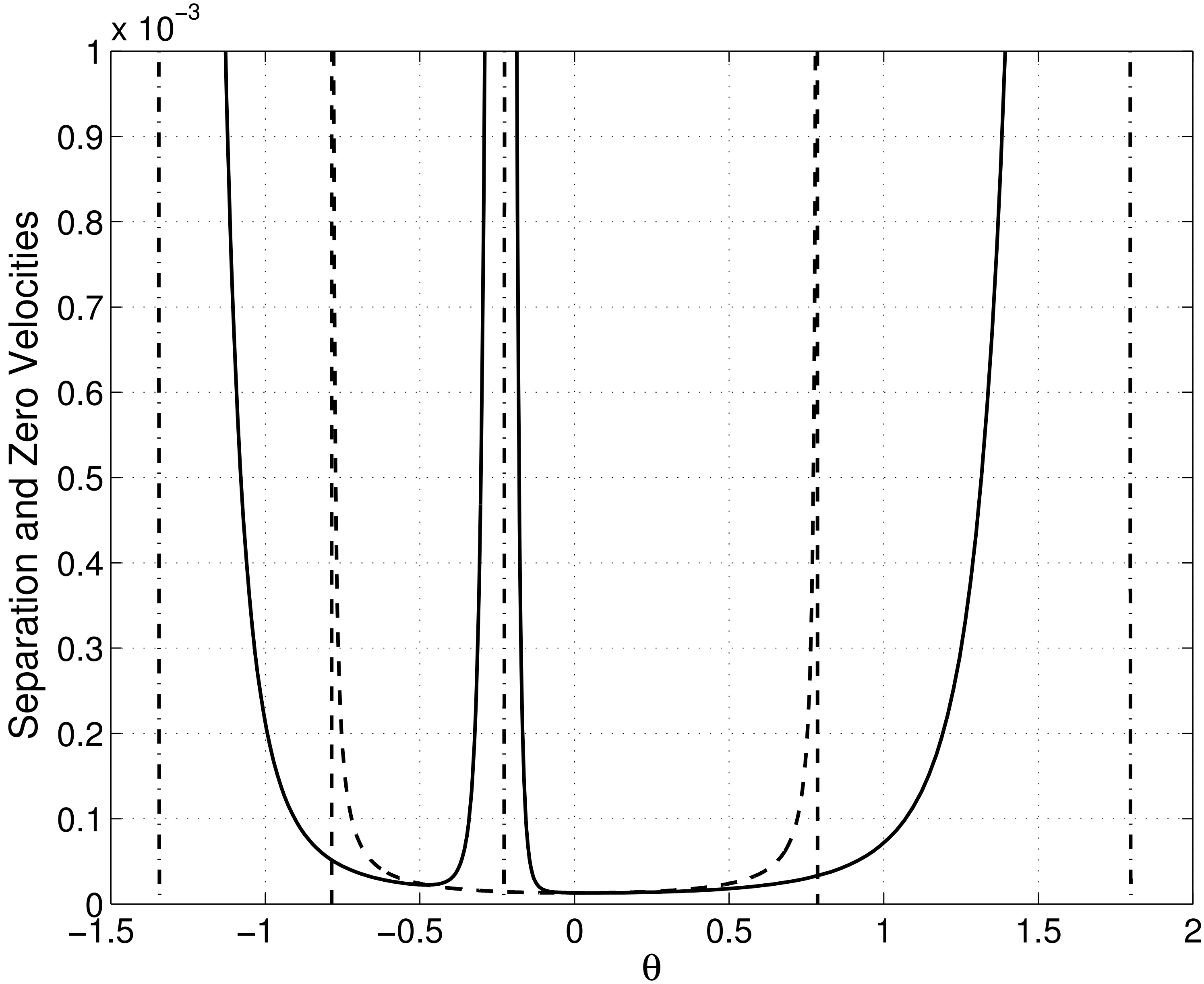
Trajectories of closest approach begin at the same separation, given k and $\bar{s}$.
Accumulated strain of two trajectories is equal.

<u>Upstream branch</u>: the spheres approach close to the compression axis and depart close to the extension axis.
<u>Downstream branch</u>: the spheres approach and depart from nearer the x-axis.

Separation s versus θ



Plots of the separation s versus θ, when $k = 3$ and $F = 10^{-4}$, for ν=0.55 (dashed) and 0.65 (solid)



Expanded view of s versus θ (solid), when $\nu = 0.60$, $k = 3$, and $F = 10^{-4}$, with curves of $\dot{s} = 0$ (dashed) and $\dot{\theta} = 0$ (dot-dashed). According with Nazockdast and Morris (2013) at left of stagnation point we have a reversing trajectory, at right a trajectory that continues in the flow direction.

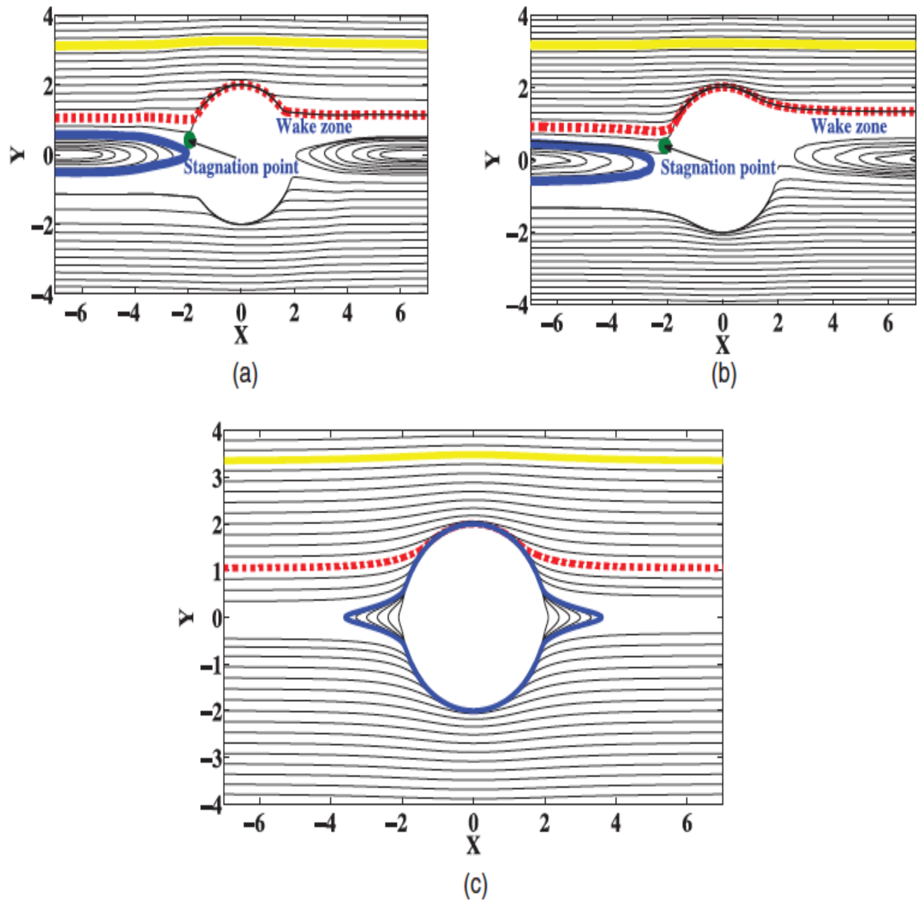
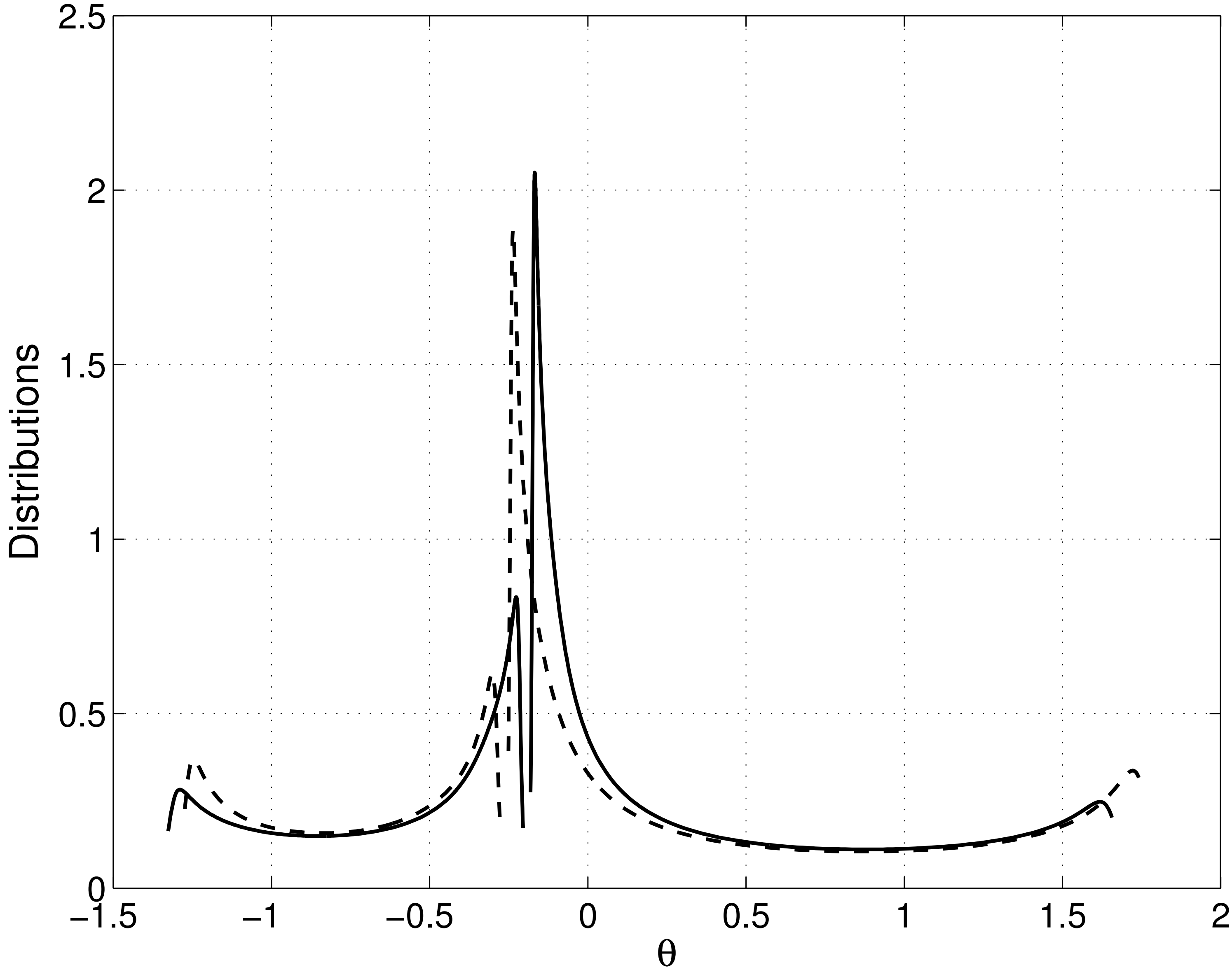
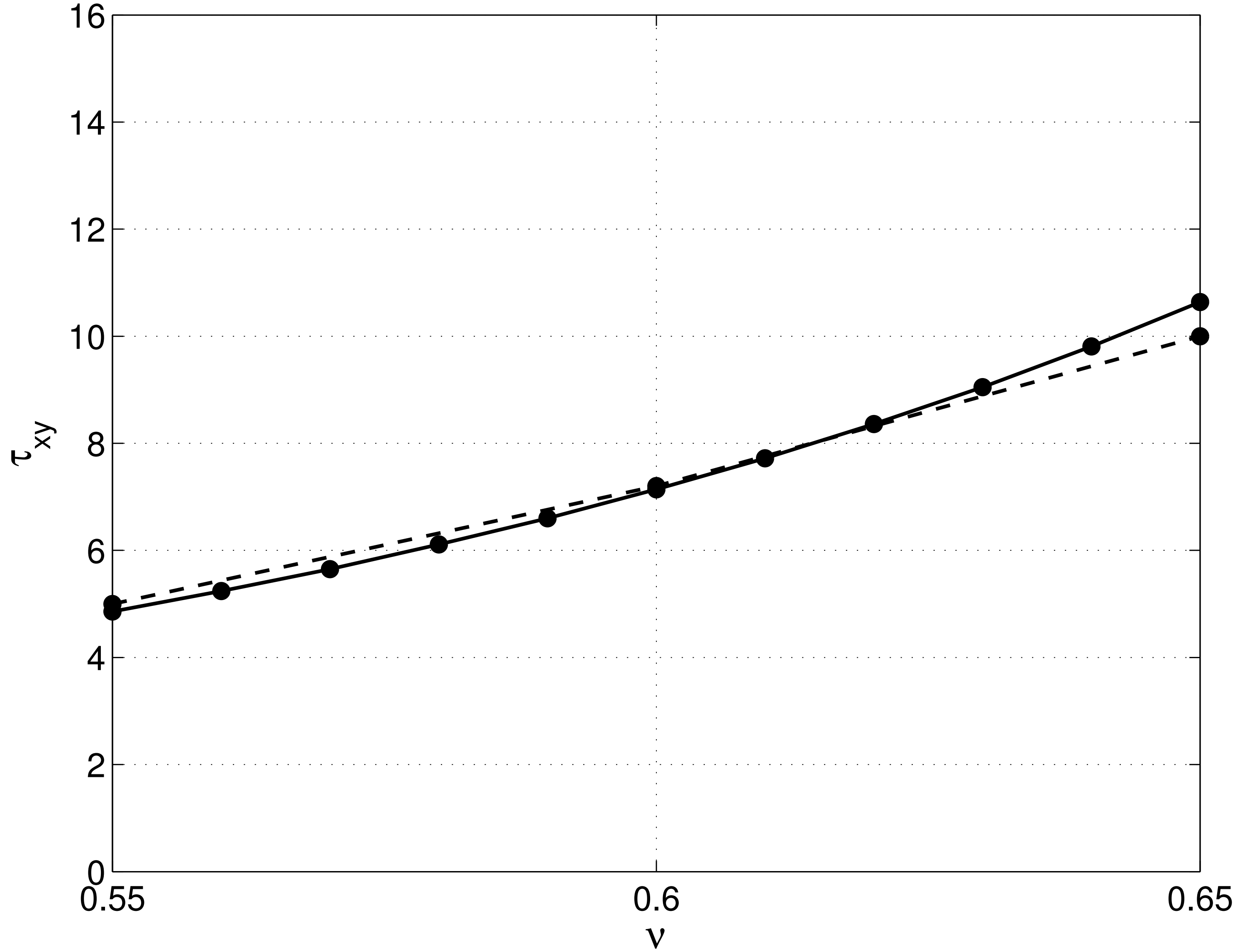


FIG. 9. Average pair trajectories in shear plane of a $\phi = 0.20$ suspension at $Pe = 100$: (a) predictions, (b) simulation results. (c) Pair trajectories of an isolated pair in simple shear flow.

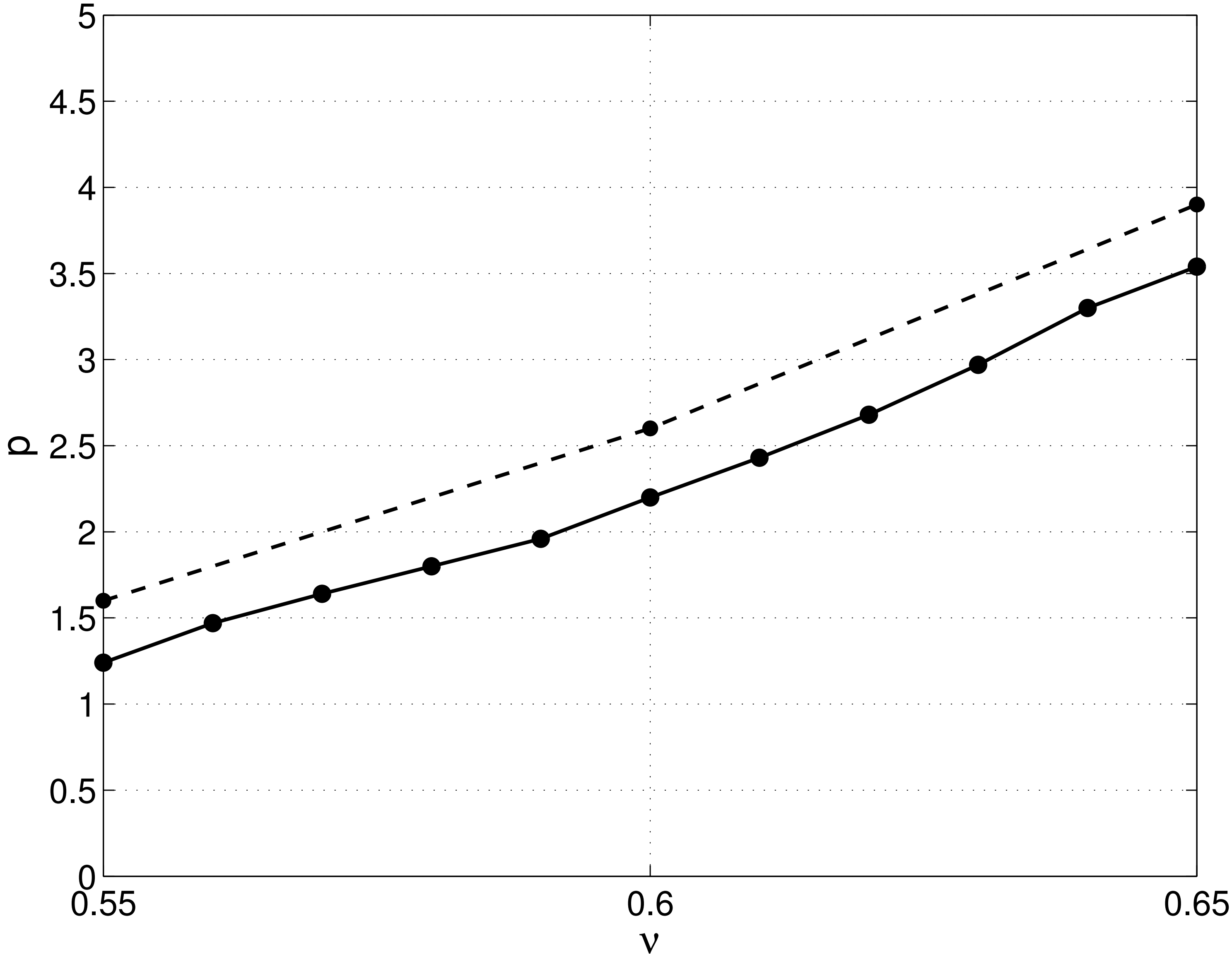
The point marked as the *stagnation point* separates reversing trajectories from those which continue in the flow direction. The average velocity magnitude is zero at this point. In the absence of Brownian fluctuations and fluctuations induced by bath particles, any pair of particles would remain stagnant in this configuration, and $g(\mathbf{r})$ would diverge at this point. Although the presence of fluctuations removes this singularity, the stagnation point is still close to the location of the maximum value of g; see Figure 6(a). The third trajectory zone contains far-field trajectories which



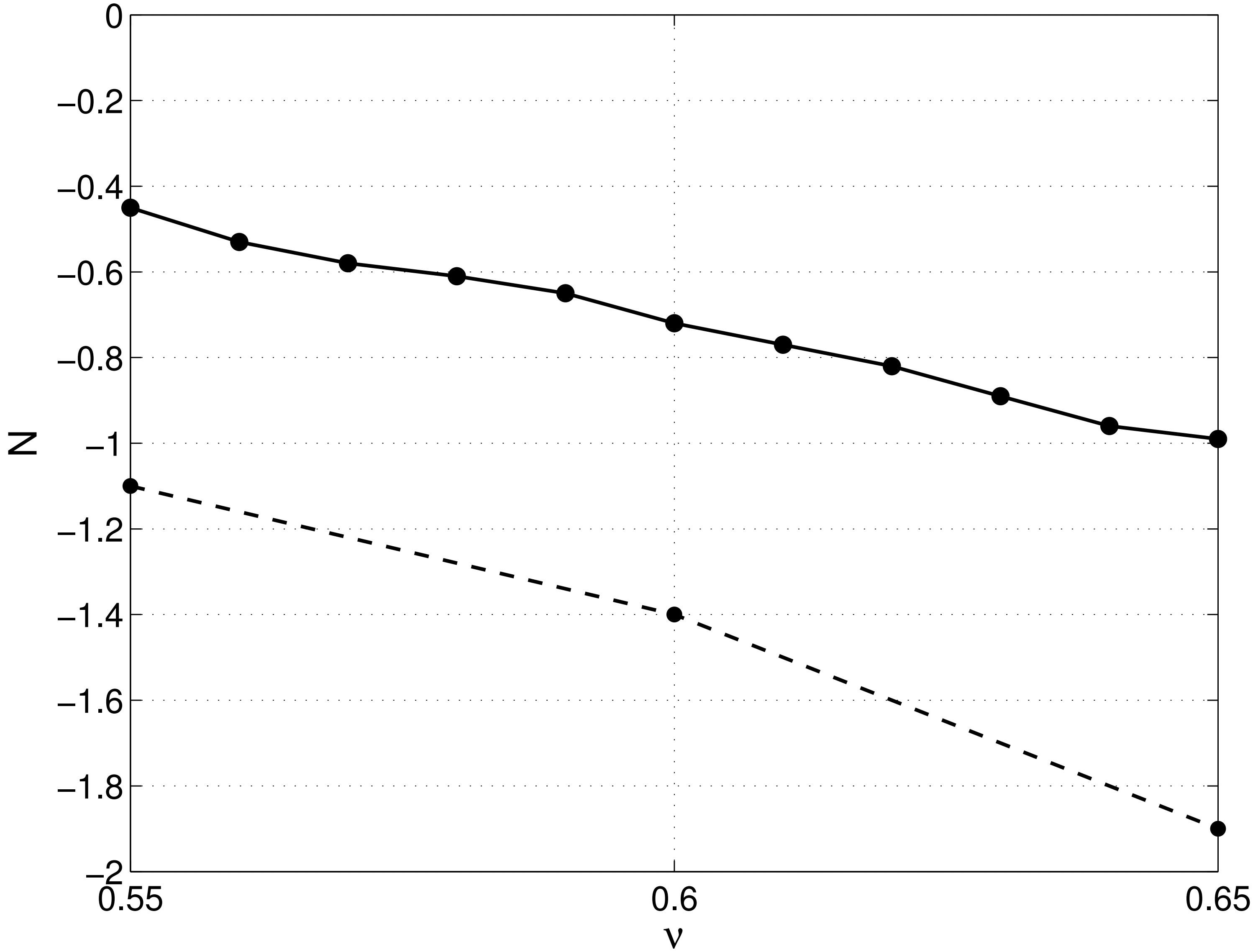
Distribution $\mathscr{A}$ versus θ, when $k = 3$ and $F = 10^{-4}$, for $\nu = 0.55$ (dashed), and 0.65 (solid). Note the peak close to the stagnation point as in Nazockdast and Morris (2013).



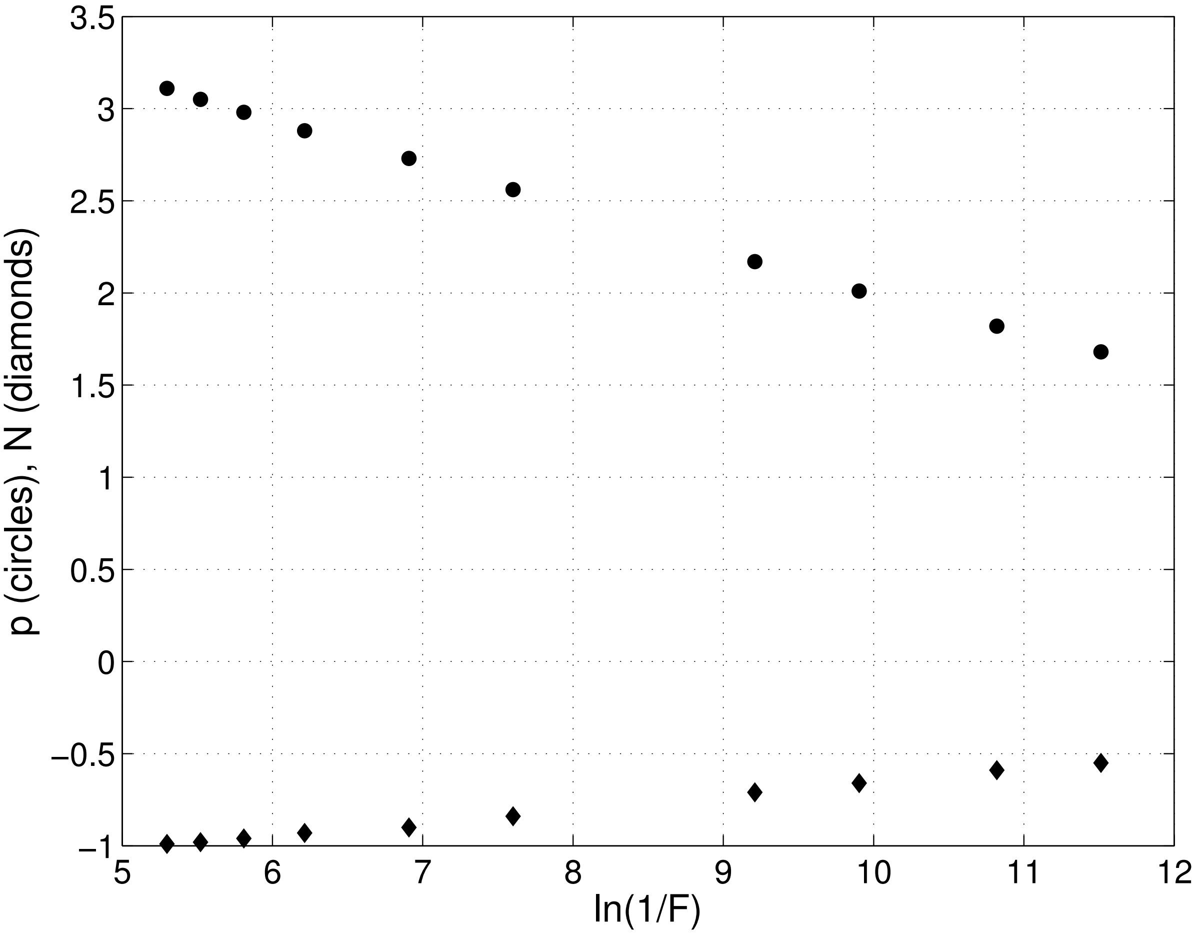
Predicted shear stress τ_{xy} versus area fraction ν (solid line connecting predicted values), with coordination number $k = 3$ and repulsive force $F = 10^{-4}$, and that measured by Singh & Nott (2000) (dashed line connecting measured values)



Predicted particle pressure p versus area fraction ν (solid line connecting predicted values), with coordination number $k = 3$ and repulsive force $F = 10^{-4}$, and that measured by Singh & Nott (2000) (dashed line connecting measured values)



Predicted normal stress difference N versus area fraction ν (solid line connecting predicted values), with coordination number $k = 3$ and repulsive force $F = 10^{-4}$, and that measured by Singh & Nott (2000) (dashed line connecting measured values)



Particle pressure p (circles) and normal stress difference N (diamonds) versus $\ln(1/F)$, for coordination number k= 3 and $\nu = 0.6$.

CONCLUSIONS

a) A rather simple model is employed to study the rheology of dense suspensions at low Reynolds number

b) Motion of a typical pair (given by an average and a fluctuation) is determined by local force equilibrium

c) Symmetry of the stress determines $\Omega^{\times} - W^{\times}$

Possible Numerical Tests:

a) Relate $\bar{s}$, ν in the anisotropic case. How different is from the isotropic prediction?

b) Measure $\Omega^{\times}$ different from $W^{\times}$?

c) Are p and N proportional to $\ln(1/F)$?

d) Can numerical simulation provide a number for k ?

Next

Extend to the 3D case: two different normal stresses

Centers of the particles not constrained to stay in the flow plane

Comparison between theory, simulations and physical experiments