Transport coefficients for suspensions of spherical particles

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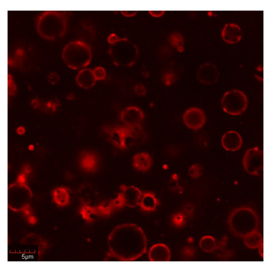
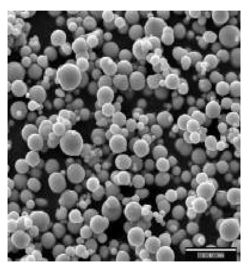
Motivation and aims

Suspensions in nature and industry

Micro:

Radius of particles
Viscosity of fluid
Number density of particles

Macroscopic properties:

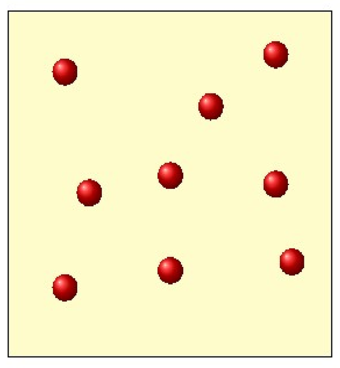
Effective viscosity
Sedimentation coefficient
Hydrodynamic factor

"The simplest" system: Suspension of spherical particles (hard spheres)

Problem: from micro to macro

Hard spheres suspension – microscopic description

Unbounded liquid,
N particles



Forces acting on suspension: $\mathbf{F}_0(\mathbf{r})$ (fluid) $\mathbf{F}_{part}(\mathbf{r})$ (particles)

Response of suspension: $\mathbf{V}_i,\ \boldsymbol{\Omega}_i,\ \sum_{i=1}^{N}\mathbf{F}_i(\mathbf{r})$

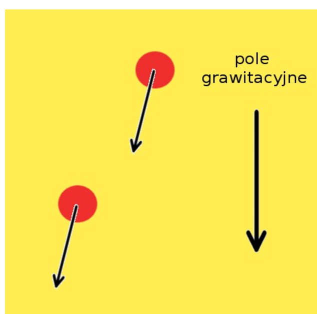
translational and angular velocity — surface forces

Stokes equations:

$$\nabla p(\mathbf{r}) - \eta\Delta\mathbf{v}(\mathbf{r}) = \mathbf{F}_0(\mathbf{r}) + \sum_{i=1}^{N}\mathbf{F}_i(\mathbf{r})$$

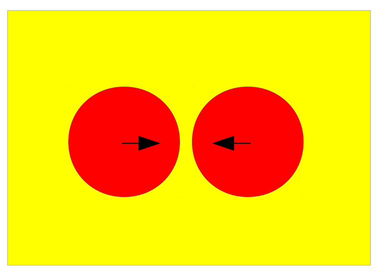
$$\nabla\cdot\mathbf{v}(\mathbf{r}) = 0$$

Hydrodynamic interactions

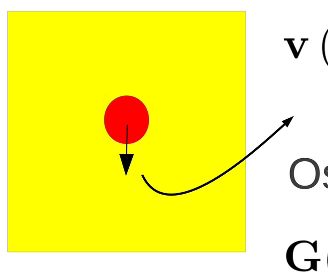


Three important features of hydrodynamic interactions:
- -strong interactions of close particles
- -long-range
- -many-body

For constant velocities asymptotically infinite drag force:



Slow decreasing of velocity field around sedimenting single particle:



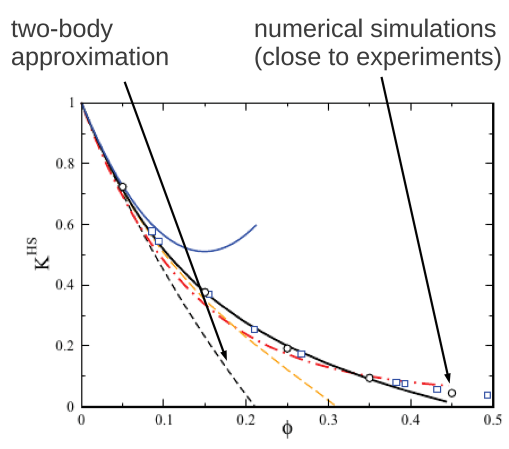
$$\mathbf{v}(\mathbf{r}) \sim \mathbf{G}(\mathbf{r})\cdot\mathbf{F}$$

Oseen tensor:

$$\mathbf{G}(\mathbf{r}) = \frac{1}{8\pi\eta}\,\frac{\mathbf{1}+\hat{\mathbf{r}}\hat{\mathbf{r}}}{r}$$

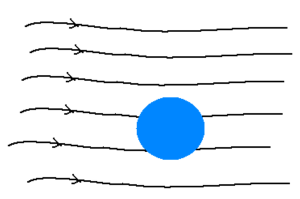
Integral over r not absolutely convergent

Many-body character:



M. Heinen, A. Banchio, and G. Nägele, J. Chem. Phys. 135, 154504 (2011).

Single particle in ambient flow:

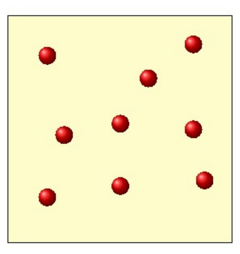


$$\mathbf{v}_0(\mathbf{r}) = \int d^3\mathbf{r}'\mathbf{G}(\mathbf{r}-\mathbf{r}')\cdot\mathbf{f}_0(\mathbf{r}')$$

$$\mathbf{f}_1(\mathbf{r}) = \int d\mathbf{r}'\mathbf{M}(\mathbf{r}-\mathbf{R}_1,\mathbf{r}'-\mathbf{R}_1)\,\mathbf{v}_0(\mathbf{r}')$$

Single freely moving particle response operator

Suspension in ambient flow:



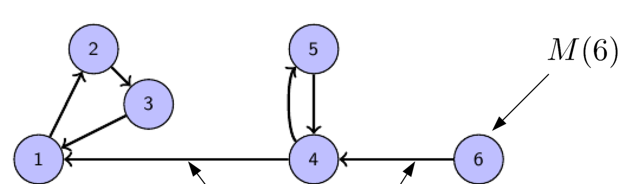
$$\mathbf{f}_i = \mathbf{M}(i)\left(\mathbf{v}_0 + \sum_{i\neq j}\mathbf{G}\mathbf{f}_j\right)$$

Scattering series

$$\mathbf{f}_i = \left(\mathbf{M}(i) + \sum_{j\neq i}\mathbf{M}(i)\mathbf{G}\mathbf{M}(j) + \sum_{j\neq i}\sum_{k\neq j}\mathbf{M}(i)\mathbf{G}\mathbf{M}(j)\mathbf{G}\mathbf{M}(k) + \ldots\right)\mathbf{v}_0$$

Green function for Stokes equations

$$M(1)GM(3)GM(2)GM(1)\times$$
$$G\times M(4)GM(5)GM(4)\times G\times M(6)$$



short range hydrodynamic interactions
(strong interactions of close particles)

long range hydrodynamic interactions (nodal line)

block structure: $S_I(C_1)$ — $S_I(C_2)$ — $S_I(C_3)$, $C_1\equiv 123$, $C_2\equiv 45$, $C_3\equiv 6$

Macroscopic description

Average force density:

$$\langle f(\mathbf{R})\rangle \equiv \left\langle \sum_i f_i\delta(\mathbf{R}-i)\right\rangle$$

Average over probability distribution for configurations of particles, thermodynamic limit

$$\langle f(\mathbf{R})\rangle = \int d^3\mathbf{R}'T(\mathbf{R},\mathbf{R}')\,v_0(\mathbf{R}')$$

Response operator for suspension in ambient flow

$$T = \sum_{b=1}^{\infty}\sum_{C_1\ldots C_b}\int dC_1\ldots dC_b\; n(C_1\ldots C_b)\,S_I(C_1)G\ldots GS_I(C_b)$$

s-particle distribution functions

Response of suspension (effective viscosity)

average velocity field of suspension

$$\langle f\rangle(\mathbf{R}) = \int d\mathbf{r}'T^{irr}(\mathbf{R},\mathbf{R}')\,\langle v\rangle(\mathbf{R}')$$

average surface dipole force

$$\langle v(\mathbf{R})\rangle = v_0(\mathbf{R}) + \int d\mathbf{r}'G(\mathbf{R},\mathbf{R}')\,\langle f(\mathbf{R}')\rangle$$

Relation between T and T^{irr} operators:

$$T = T^{irr}\left(1 - GT^{irr}\right)^{-1}$$

Felderhof, Ford, Cohen (1982):

$$T^{irr} = \sum_{g=1}^{\infty}\sum_{C_1\ldots C_g}\int dC_1\ldots dC_g b(C_1|\ldots|C_g)S_I(C_1)G\ldots GS_I(C_g)$$

Effective viscosity coefficient is given directly by the response operator T^{irr}

$$b(C) = n(C)$$
$$b(C_1|\ldots|C_k|C_{k+1}|\ldots|C_g) = b(C_1|\ldots|C_kC_{k+1}|\ldots|C_g) - b(C_1|\ldots|C_k)b(C_{k+1}|\ldots|C_g)$$

Renormalization

Ring expansion (2011):

$$T^{irr} = \sum_{b=1}^{\infty}\sum_{C_1\ldots C_b}\int dC_1\ldots dC_bH(C_1|\ldots|C_b)S_I(C_1)G_{\rm eff}\ldots G_{\rm eff}S_I(C_b)$$

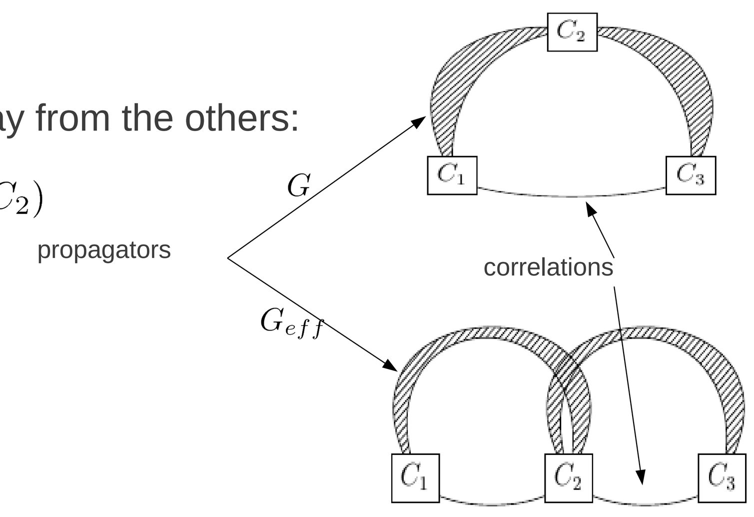
Block correlation functions (recurrence formula):

$$\mathrm{b}(C_1|\ldots|C_b) = \sum_{r=1}^{b-1}\sum_{1=i_1<i_2<\ldots<i_{r+1}=b} H(C_{i_1}|\ldots|C_{i_{r+1}})n(\{C_{i_1}\ldots C_{i_2}\}\setminus\{C_{i_1}C_{i_2}\})\ldots n\left(\{C_{i_r}\ldots C_{i_{r+1}}\}\setminus\{C_{i_r}C_{i_{r+1}}\}\right)$$

When the middle group goes away from the others:

Cluster expansion: $b(C_1|C_2|C_3) \longrightarrow b(C_1|C_3)\,b(C_2)$

Ring expansion: $H(C_1|C_2|C_3) \longrightarrow 0$



Two important differences:
-propagator
-volume of integration

Approximate method of calculations of transport properties

Repeating structures in T^{irr}

Felderhof, Ford, Cohen (1982) (Mayer insteadd of h):

$$T^{irr} = T^{irr}_{CM}\left(1 - [hG]\,T^{irr}_{CM}\right)^{-1}$$

Clausius-Mossotti operator

Clausius-Mossotti approximation:

$$T^{irr}_{CM} \approx nM$$

renormalized Clausius-Mossotti operator

$$T^{irr} = T^{irr}_{RCM}\left(1 - [hG_{\rm eff}]\,T^{irr}_{RCM}\right)^{-1}$$

Approximate method formulated in terms of approximation for T^{irr}_{RCM}
$G \Longrightarrow G_{\rm eff}$

Generalized Clausius-Mossotti approximation:

$$T^{irr}_{RCM} \approx nB$$

(two-body hydrodynamic interactions incomplete – the same as in δγ scheme (1983))

One-ring approximation (fully takes into account two-body hydrodynamic interactions)

Input:
-volume fraction
-two-body correlation function (PY); (three-particle correlation function by two body correlation function (Kirkwood))
-two-body hydrodynamic interactions