Transport properties of suspensions of spherical particles

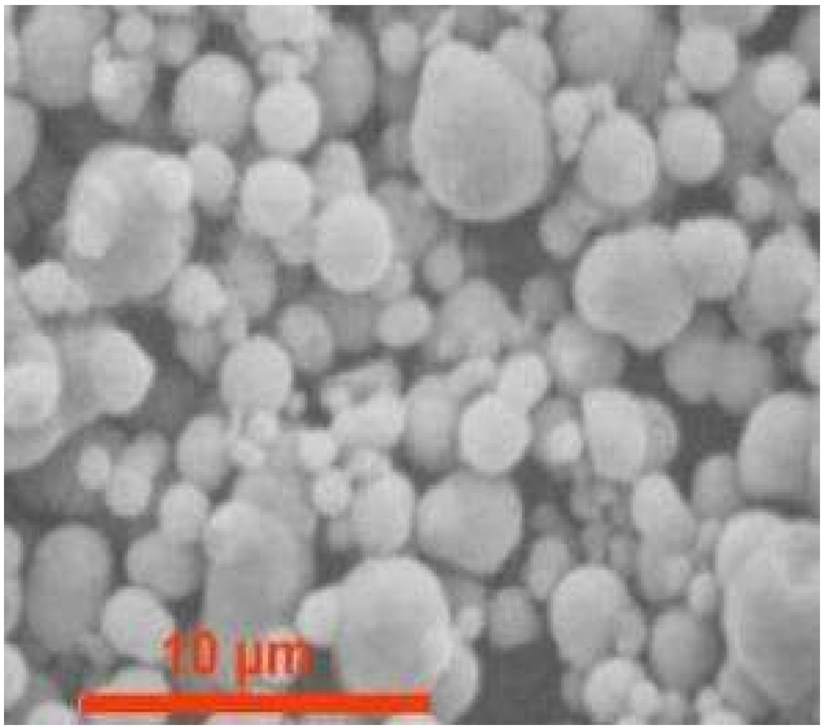
Karol Makuch

UNIVERSITAS VARSOVIENSIS

27.11.2015, IChF PAN

Introduction - suspensions

minute particles in liquid



milk, blood,...

Liquid:

-temperature T

-viscosity μ

-density of the fluid ρ_f

Particles:

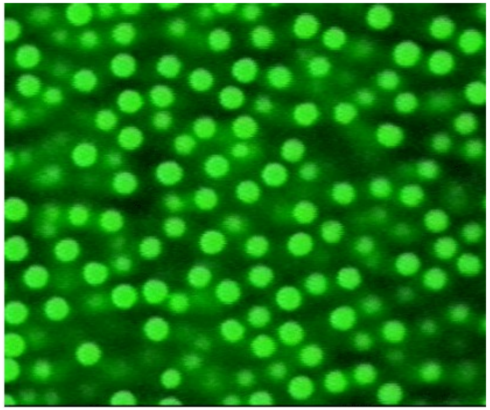
-radius a

-density of material ρ_p

-volume fraction ϕ

Goal of the research

Suspension of spherical particles

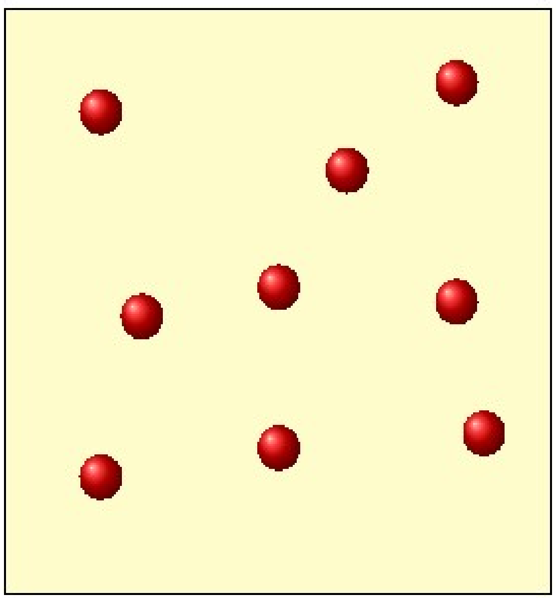


Transport properties (short time):
-effective viscosity
-sedimentation coefficient
-diffusion coefficient

Over 100 years of theoretical research - still an open question

Hard-sphere suspension

Unbounded liquid,
N particles in configuration $X \equiv \mathbf{R}_1, \ldots, \mathbf{R}_N$



Stokes equations:

$$\begin{aligned} \nabla p\left(\mathbf{r}\right) - \eta \Delta \mathbf{v}\left(\mathbf{r}\right) &= 0 \\ \nabla \cdot \mathbf{v}\left(\mathbf{r}\right) &= 0 \end{aligned}$$

Stick boundary conditions,

$$\mathbf{v}(\mathbf{r}) \rightarrow \mathbf{v}_0(\mathbf{r}) \quad \textit{for} \quad r \rightarrow \infty$$

Aristotelian world...

Stokes (1851)

Flow around sedimenting particle

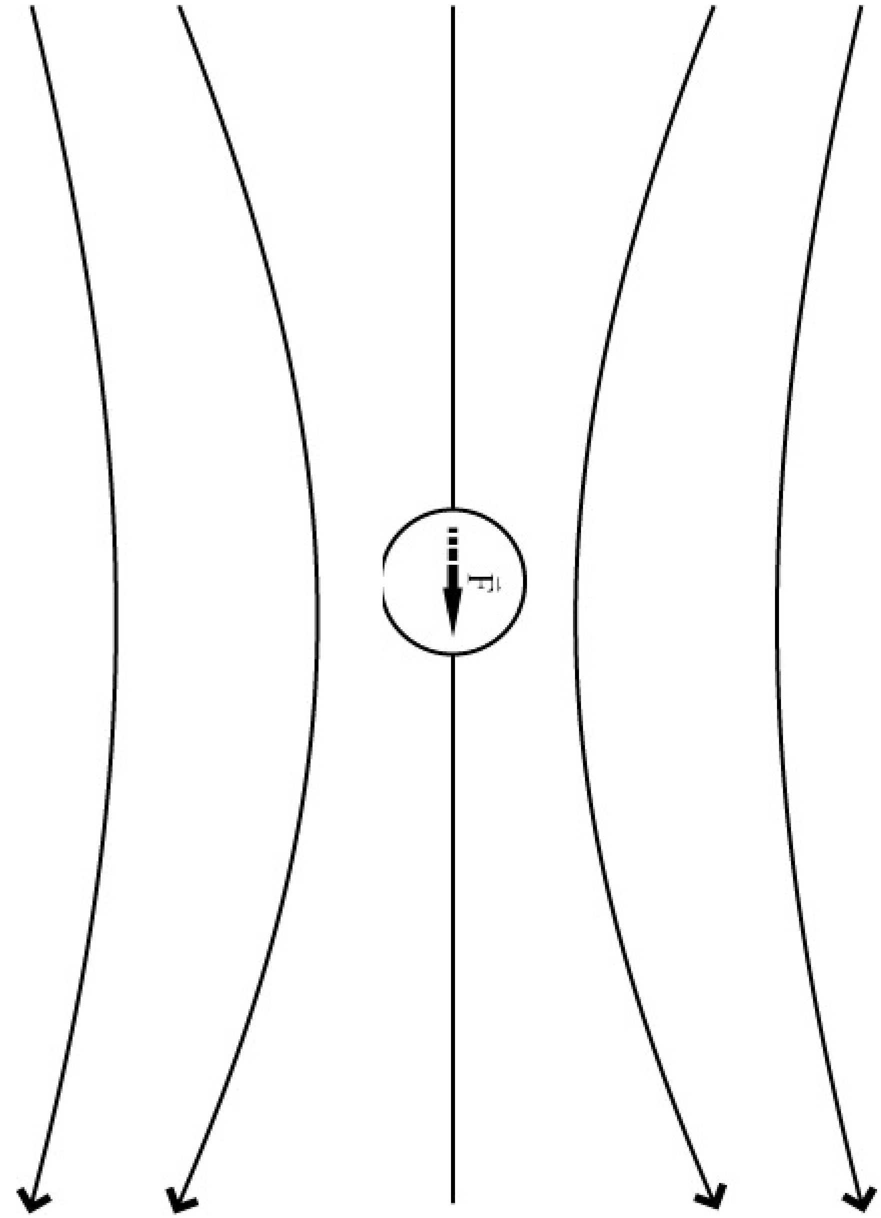
External force acting on the particle

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

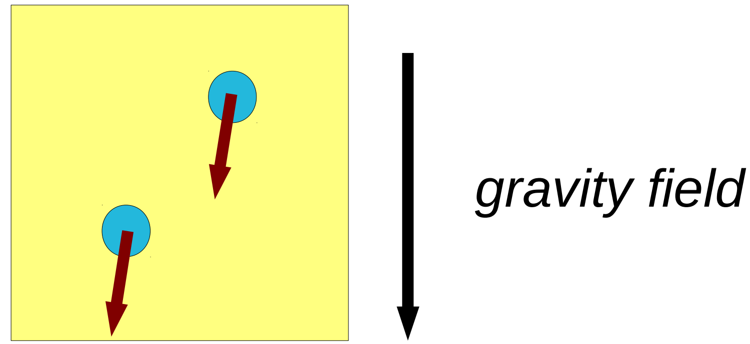
at the distance

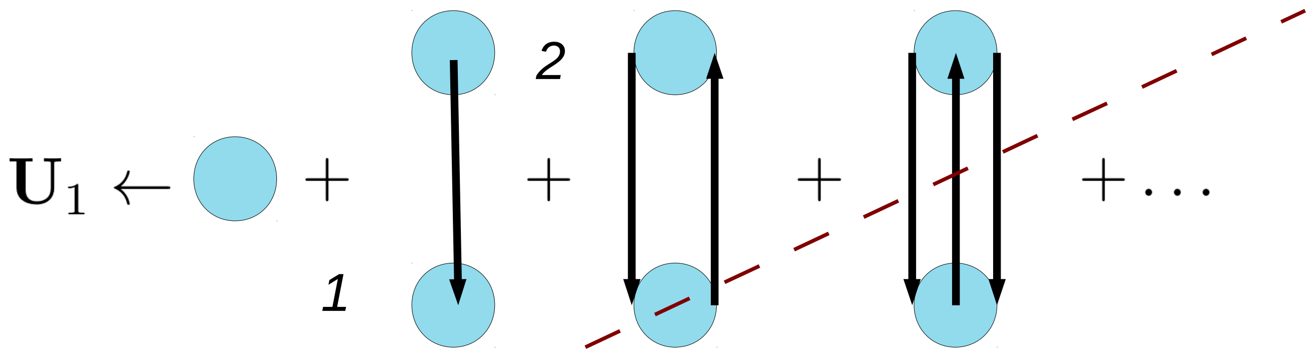
Oseen tensor - (Green function)

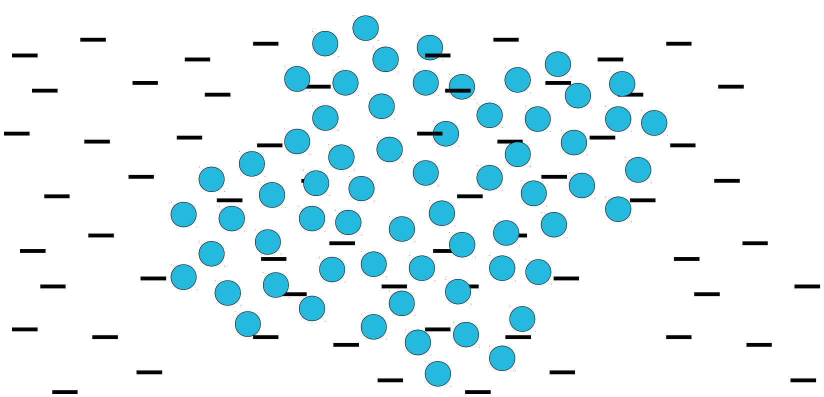
$$\mathbf{G}(\mathbf{r}) = \frac{1}{8\pi\eta}\frac{\mathbf{1} + \hat{\mathbf{r}}\hat{\mathbf{r}}}{r}$$



Hydrodynamic interactions – Smoluchowski (1911)







Long-range:

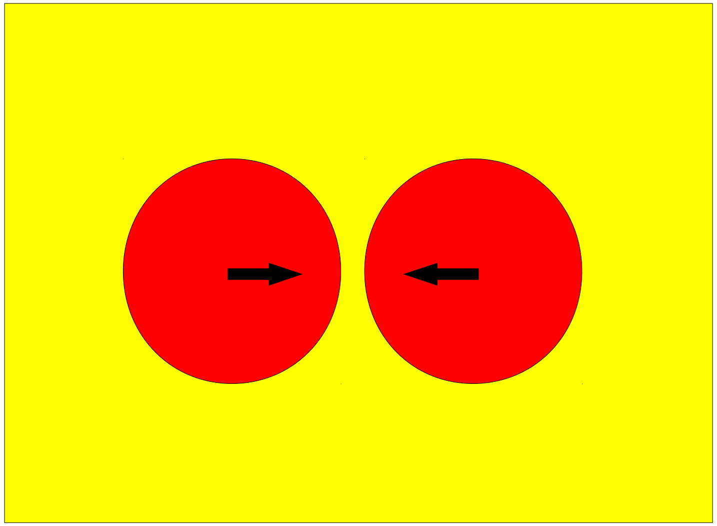
$$\int d^3r \left|\mathbf{G}(\mathbf{r})\right| = \infty$$

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

Well defined expression for effective viscosity?

Hydrodynamic interactions

Strong interactions of close particles



For constant velocities asymptotically infinite drag force
(Jeffrey, Onishi (1984))

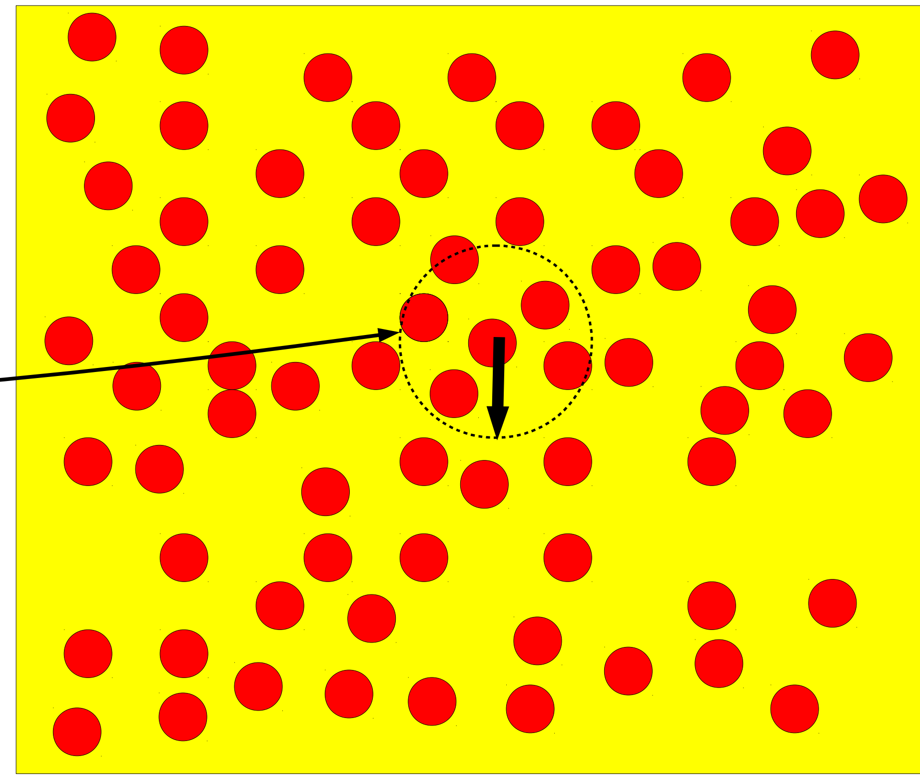
(Lubrication force)

Effective Green function

Flow caused by force acting on particles in the area

total force acting on particles in the area

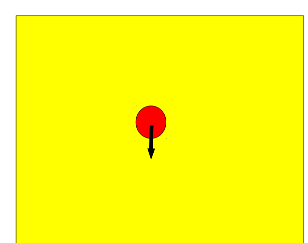
$$\mathbf{v}\left(\mathbf{r}\right) \sim \mathbf{G}_{\mathrm{eff}}\left(\mathbf{r}\right)\mathbf{F}$$



effective Green function (effective propagator):

$$\mathbf{G}_{\mathrm{eff}}(\mathbf{r}) \sim \frac{1}{8\pi\eta_{\mathrm{eff}}}\frac{\mathbf{1}+\hat{\mathbf{r}}\hat{\mathbf{r}}}{r} = \frac{\eta}{\eta_{\mathrm{eff}}}\mathbf{G}(\mathbf{r})$$

at the distance



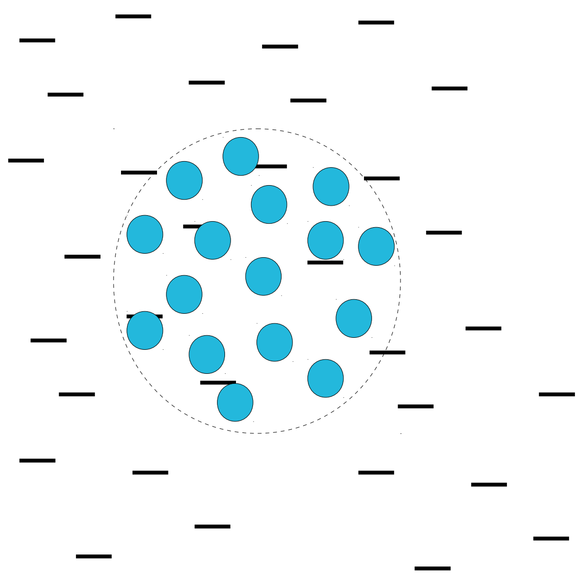
$$\mathbf{v}\left(\mathbf{r}\right) \sim \mathbf{G}\left(\mathbf{r}\right)\cdot\mathbf{F}$$

Transport properties – history and scattering series

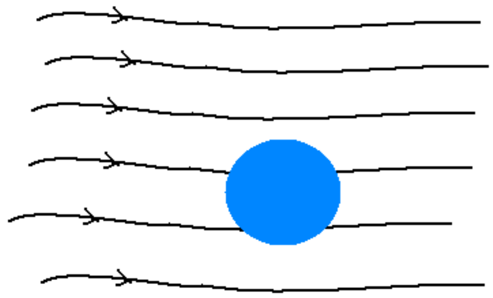
Einstein 1905 (corrected):

$$\eta_{eff} = \eta(1 + \frac{5}{2}\phi)$$

$$\phi = \frac{4}{3}\pi a^3 n$$



Single particle problem in shear flow

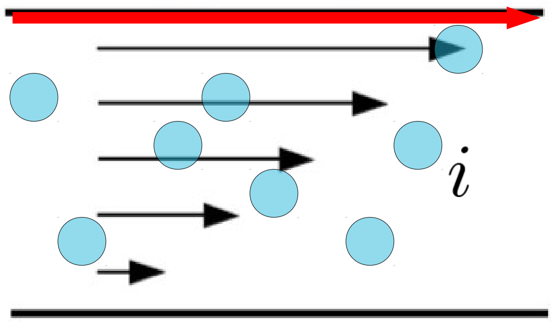


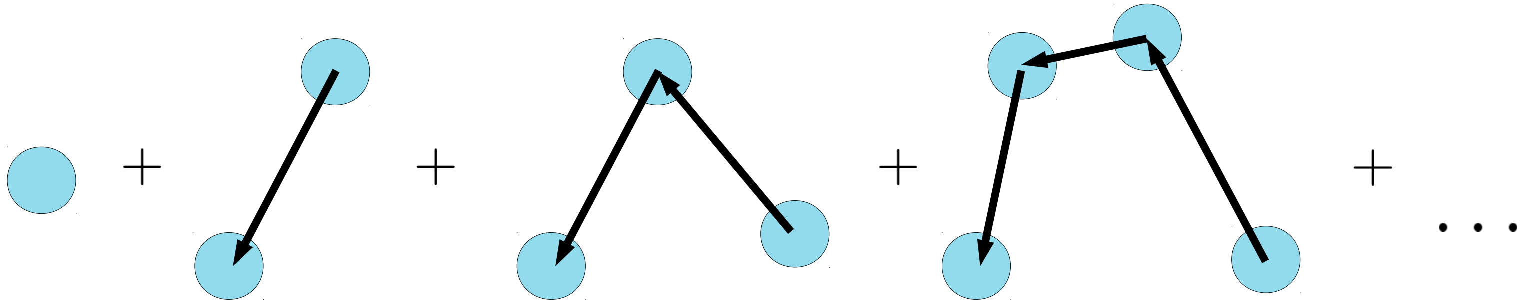
- *Finite system*
- *Hydrodynamic interactions neglected (no reflections)*
- *Diluted suspensions (volume fraction below about 3%)*

Beyond diluted suspensions

Saito (1950):

-extension of Einstein work on mean-field level



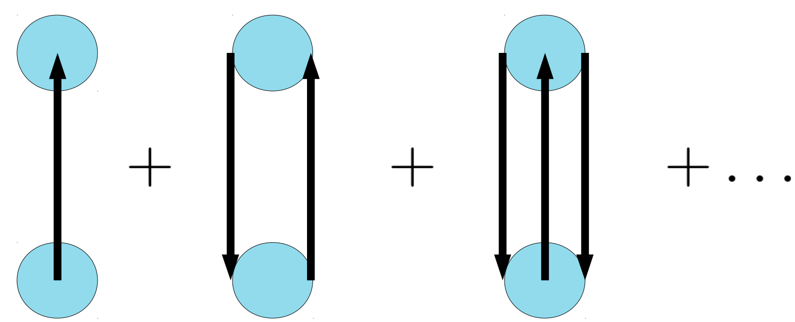


$$\frac{\eta_{eff}}{\eta} = \frac{1 + \frac{3}{2}\phi}{1 - \phi}$$

non-absolutely convergent integrals!

Two-particle hydrodynamic interactions (1963)

$$\frac{\eta_{eff}}{\eta} = 1 + \frac{5}{2}\phi + a_2\phi^2 + \dots$$



absolute convergence

$$\int d^3r \left|\mathbf{G}(\mathbf{r})\right| = \infty$$

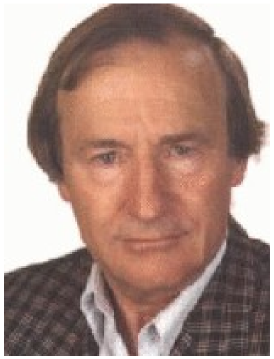
(well defined expression on two-body level)

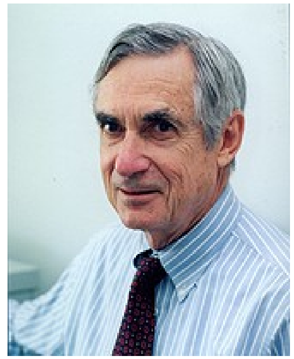
Peterson, Fixman (1963): $a_2 \approx 4.31784$

Batchelor, Green (1972): $a_2 \approx 5.2$ (ad hoc renormalization)

Problem with long-range HI still not solved

1982 – problem of long-range HI solved





B. U. Felderhof,[1] G. W. Ford,[2] and E. G. D. Cohen[3]

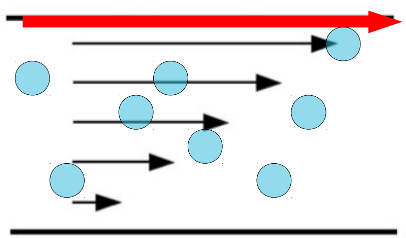
Received August 24, 1981

We derive a cluster expansion for the electric susceptibility kernel of a dielectric suspension of spherically symmetric inclusions in a uniform background. This also leads to a cluster expansion for the effective dielectric constant. It is shown that the cluster integrals of any order are absolutely convergent, so that the dielectric constant is well defined and independent of the shape of the sample in the limit of a large system. We compare with virial expansions derived earlier in

dielectric <=> suspension

Response of suspension (effective viscosity)

Landau's book: Viscosity from the following relation:



average velocity field of suspension

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

average surface force (dipole)

viscosity operator

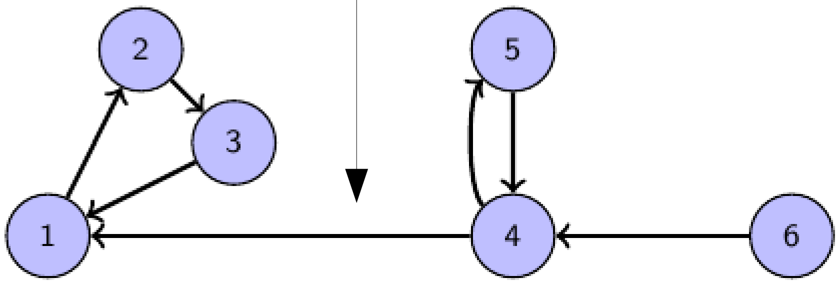
Effective viscosity coefficient is given directly by the response operator T^{irr}

Felderhof, Ford, Cohen – cluster expansion (1982)

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

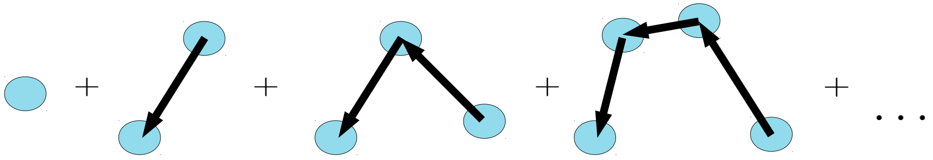
Oseen tensor: $G = \frac{1}{8\pi\eta} \frac{\mathbf{1} + \hat{\mathbf{r}}\hat{\mathbf{r}}}{r}$

Information about distribution of particles in space



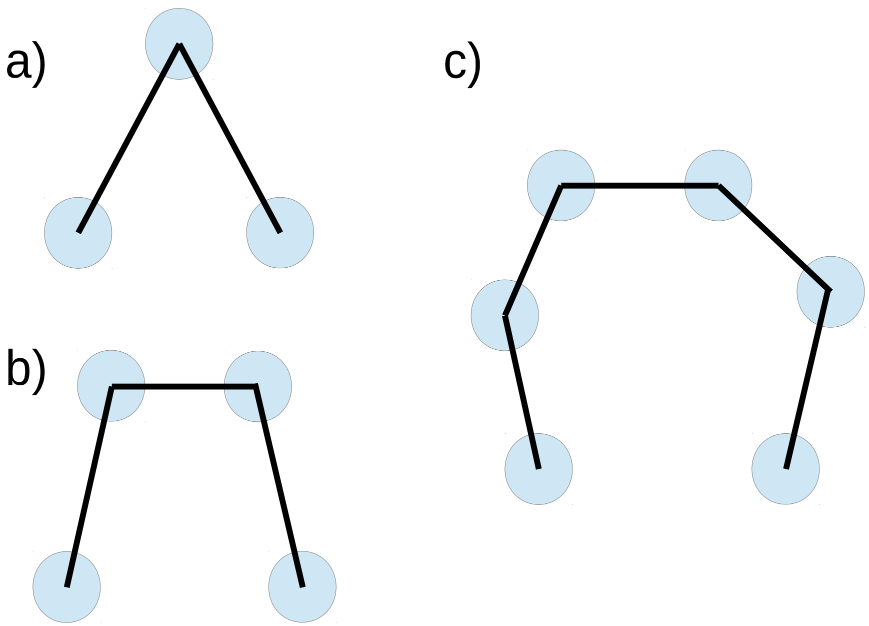
Felderhof, Ford and Cohen also identified terms, which lead to Saito formula for effective viscosity:

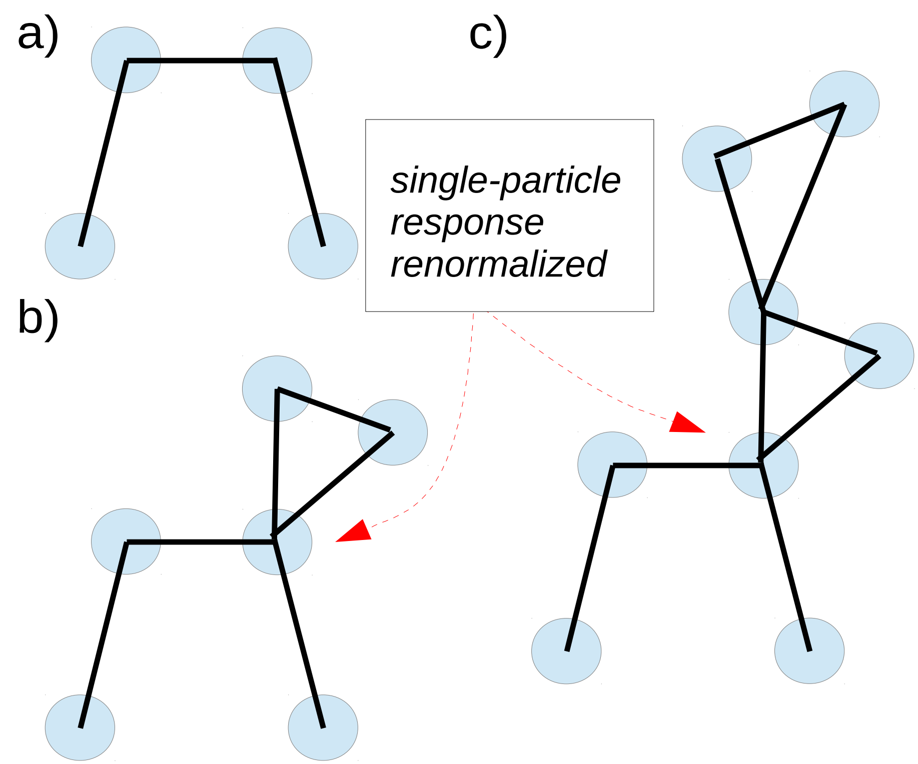
$$\frac{\eta_{eff}}{\eta} = \frac{1 + \frac{3}{2}\phi}{1 - \phi}$$



Beenakker-Mazur method (1983)

Idea of the method – resummation of certain class of hydrodynamic interactions – 'ring-selfcorrelations'





Beenakker and Mazur method

Beenakker and Mazur scheme – expansion in density fluctuations (1983). The state of the art statistical physics theory for short times properties of suspension nowadays

- ✔ *Many-body character*
- ✔ *Long-range character*
- ✘ *Strong interactions of close particles (lubrication)*

No satisfactory statistical physics method including the above three features.

Numerical simulation shows that lubrication is indispensable!

To construct the method taking into consideration lubrication is an open problem of theoretical physics.

Our approach – renormalization of the propagator

short-range hydrodynamic interaction

Cluster expansion (1982):

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

block distribution function (configurations of particles)

Oseen tensor (pure liquid):

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

Ring expansion (2015):

$$T^{irr} = \sum_{g=1}^{\infty} \sum_{C_1 \ldots C_g} \int dC_1 \ldots dC_g H(C_1|\ldots|C_g) S_I(C_1) G_{\text{eff}} \ldots G_{\text{eff}} S_I(C_g)$$

block correlation function
(configurations of particles);
H=b for g=1,2,
H different from b for g>2.

Effective Green function:

$$\mathbf{G}_{\text{eff}}(\mathbf{r}) \sim \frac{\eta}{\eta_{\text{eff}}} \mathbf{G}(\mathbf{r})$$

convergence

Generalization of Clausius-Mossotti approximation

Constructing approximate method by carrying over approximation from cluster expansion to ring expansion with the following modification:

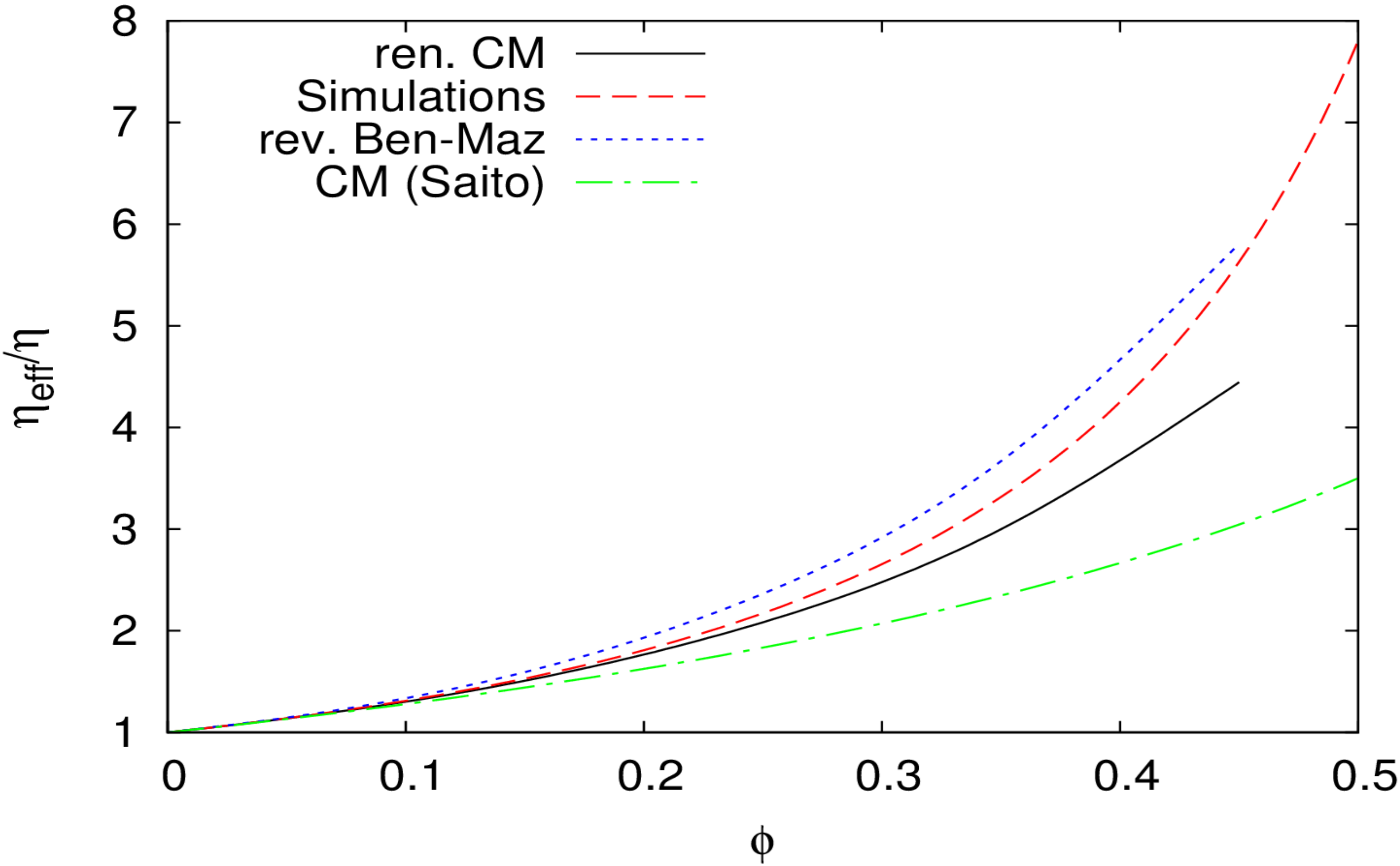
$$G \Longrightarrow G_{\mathrm{eff}}$$

Clausius-Mossotti (Saito) approximation $\Longrightarrow$ *Generalized (renormalized) Clausius-Mossotti approximation*

(two-body hydrodynamic interactions incomplete – the same as in Beenakker and Mazur scheme)

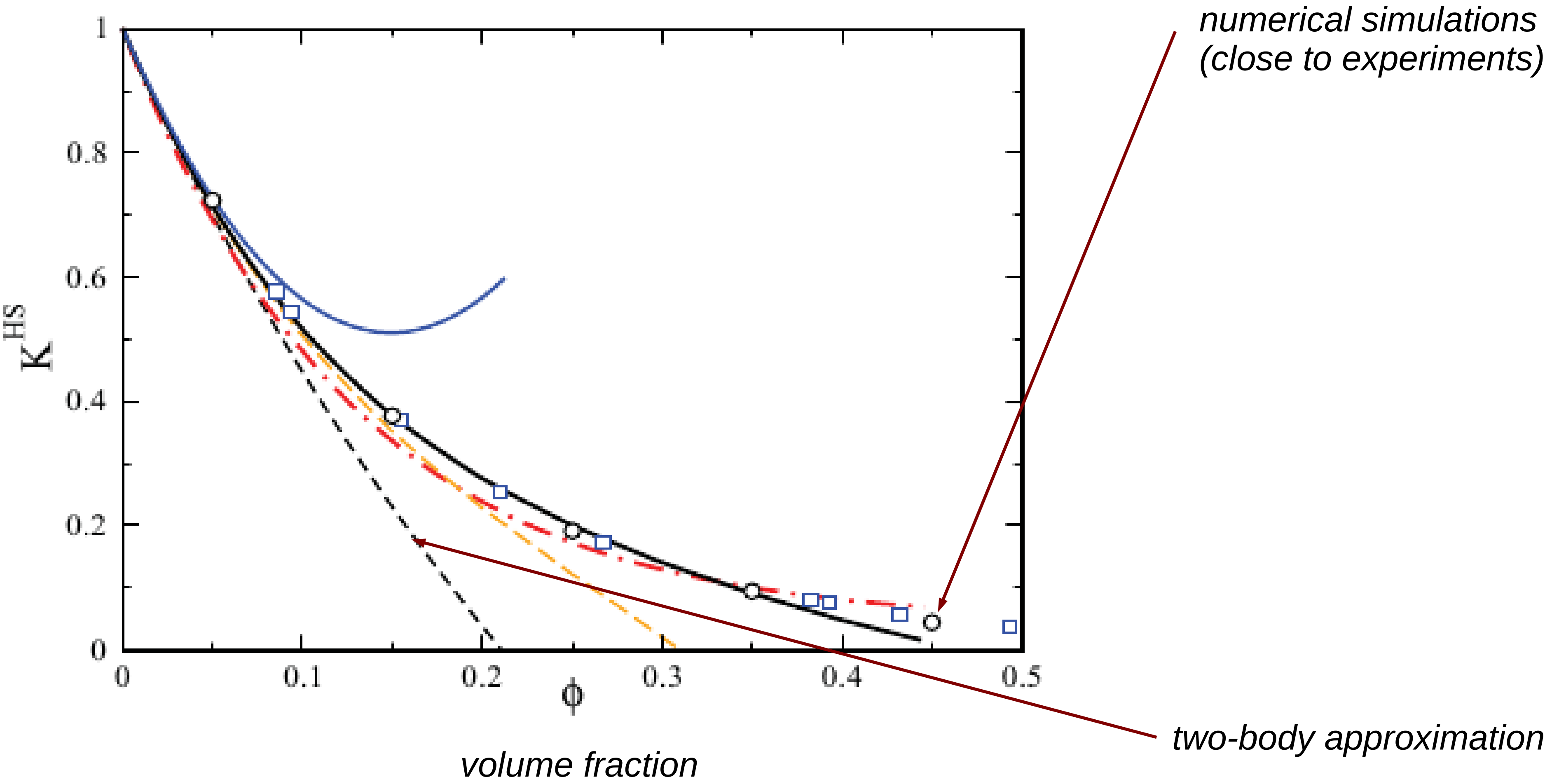
Volume fraction, two-body correlation function $\Longrightarrow$ *transport properties*

Effective viscosity



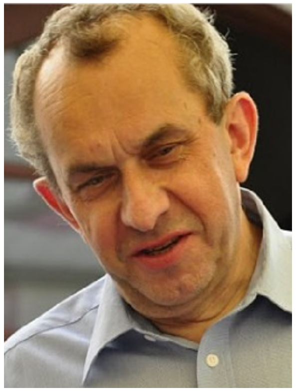
K.M. Phys. Rev. E, 92, 042317 (2015)

Sedimentation coefficient



Summary

- Long-range, many-body hydrodynamic interactions and strong interactions of close particles are important in suspensions (still an open problem)
- Rigorous ring expansion can grasp all of the above features (opposite to Beenakker-Mazur method)
- Generalized Clausius-Mossotti approximation (two-body hydrodynamic interactions not fully taken; comparable to Beenakker-Mazur scheme)

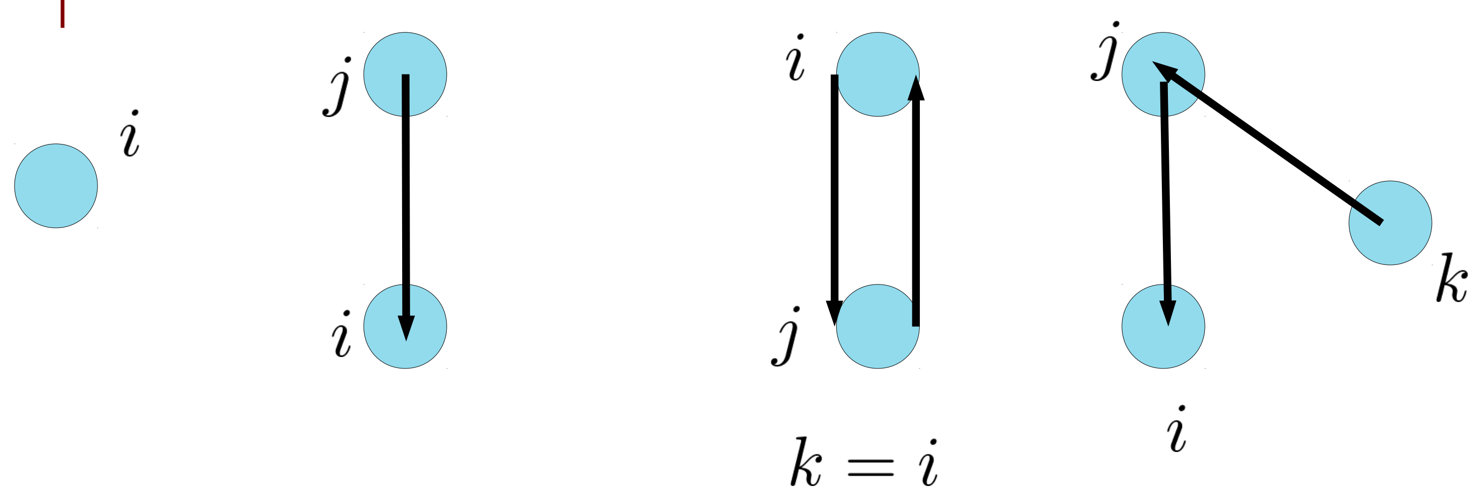


Under suspervision (in years 2005-2011) of Bogdan Cichocki, Univeristy of Warsaw

Scattering series

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

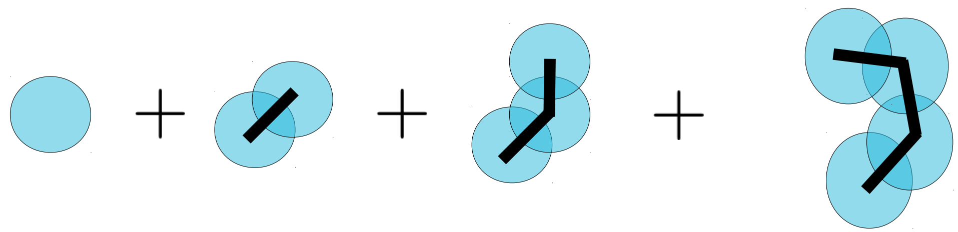
$$\mathbf{G}(\mathbf{r}) = \frac{1}{8\pi\eta} \frac{\mathbf{1} + \hat{\mathbf{r}}\hat{\mathbf{r}}}{r}$$



suspension <=> dielectrics <=> other systems

Felderhof, Ford, Cohen – microscopic explanation of Clausius-Mossotti (Saito) formula (1983)

$\mathbf{T}^{irr} \leftarrow$



$+ \dots$

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

The following definition

$$\mathbf{T}^{irr}_{CM} = \mathbf{T}^{irr} \left(1 + [h\mathbf{G}] \, \mathbf{T}^{irr} \right)^{-1}$$

and approximate closure relation

$$\mathbf{T}^{irr}_{CM} \approx n_1 \hat{\mathbf{M}}$$

lead to Saito formula

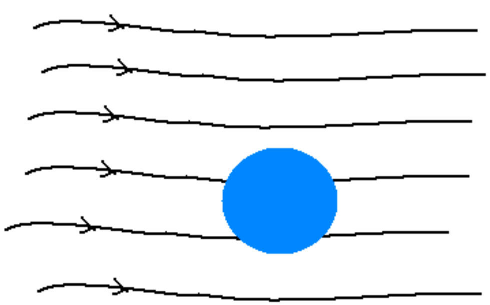
$$\frac{\eta_{eff}}{\eta} = \frac{1 + \frac{3}{2}\phi}{1 - \phi}$$

Single particle

Lamb (1895) $\mathbf{v}^{+}_{lm\sigma}(\mathbf{r})$

$l = 1, 2, \ldots, \infty$
$m = -l, \ldots, l$
$\sigma = 0, 1, 2$

Single particle in ambient flow $\mathbf{v}_0(\mathbf{r})$



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

Single particle operator
(Felderhof 1976)

Surface force density
(Cox Brenner (1967); Mazur, Bedeaux (1974))

$$\mathbf{v}(\mathbf{r}) = \mathbf{v}_0(\mathbf{r}) + \int d^3\mathbf{r}' \mathbf{G}(\mathbf{r} - \mathbf{r}') \cdot \mathbf{f}_1(\mathbf{r}')$$

Oseen tensor:

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